



## INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

<p>(51) International Patent Classification 5 :  <b>C07K 13/00, C12N 15/29  A01H 5/00, 5/10, 1/00  C12N 1/21 // (C12N 1/21  C12R 1/01)</b> </p>		<p><b>A1</b></p>	<p>(11) International Publication Number: <b>WO 91/04270</b></p>
			<p>(43) International Publication Date: <b>4 April 1991 (04.04.91)</b></p>
<p>(21) International Application Number: <b>PCT/AU90/00430</b></p> <p>(22) International Filing Date: <b>19 September 1990 (19.09.90)</b></p> <p>(30) Priority data:  <b>PJ 6441 20 September 1989 (20.09.89) AU</b></p> <p>(71)(72) Applicant and Inventor (<i>for all designated States except US</i>): <b>COMMONWEALTH SCIENTIFIC AND INDUSTRIAL RESEARCH ORGANISATION [AU/AU]; Limestone Avenue, Campbell, ACT 2601 (AU).</b></p> <p>(72) Inventors: and</p> <p>(75) Inventors/Applicants (<i>for US only</i>): <b>COLMAN, Peter, Malcolm [AU/AU]; 30a Hawthorn Glen, Hawthorn, VIC 3122 (AU). LAWRENCE, Michael, Colin [ZA/AU]; 35 Finmere Crescent, Upper Ferntree Gully, VIC 3156 (AU). VARGHESE, Joseph, Noozhumurry [AU/AU]; 62 Newry Street, North Fitzroy, VIC 3068 (AU). HALL, Timothy, Couzens [US/US]; 1044 Rose Circle, College Station, TX 77840 (US). BUSTOS, Mauricio, Martin [AR/US]; 1418 Magnolia Drive, College Station, TX 77840 (US).</b></p>		<p>(74) Agent: <b>SANTER, Vivien; Griffith Hack &amp; Co, 601 St Kilda Road, Melbourne, VIC 3004 (AU).</b></p> <p>(81) Designated States: <b>AT (European patent), AU, BE (European patent), BR, CA, CH (European patent), DE (European patent)*, DK (European patent), ES (European patent), FR (European patent), GB (European patent), IT (European patent), JP, LU (European patent), NL (European patent), SE (European patent), SU, US.</b></p> <p><b>Published</b>  <i>With international search report.</i></p>	
<p><b>(54) Title: MODIFIED SEED STORAGE PROTEINS</b></p> <p><b>(57) Abstract</b></p> <p>The invention provides modified plant storage proteins, in which the modification is effected in the primary structure of the protein, and the tertiary and quaternary structure of the protein is retained. The site for modification is selected by reference to the three-dimensional structure of the protein, which has been newly established by the inventors. Modified DNA molecules, vectors, transgenic plants, and parts and products thereof are also claimed.</p>			

### DESIGNATIONS OF "DE"

Until further notice, any designation of "DE" in any international application whose international filing date is prior to October 3, 1990, shall have effect in the territory of the Federal Republic of Germany with the exception of the territory of the former German Democratic Republic.

#### FOR THE PURPOSES OF INFORMATION ONLY

Codes used to identify States party to the PCT on the front pages of pamphlets publishing international applications under the PCT.

AT	Austria	ES	Spain	MC	Monaco
AU	Australia	FI	Finland	MG	Madagascar
BB	Barbados	FR	France	ML	Mali
BE	Belgium	GA	Gabon	MR	Mauritania
BF	Burkina Fasso	GB	United Kingdom	MW	Malawi
BG	Bulgaria	GR	Greece	NL	Netherlands
BJ	Benin	HU	Hungary	NO	Norway
BR	Brazil	IT	Italy	PL	Poland
CA	Canada	JP	Japan	RO	Romania
CF	Central African Republic	KP	Democratic People's Republic of Korea	SD	Sudan
CG	Congo	KR	Republic of Korea	SE	Sweden
CH	Switzerland	LI	Liechtenstein	SN	Senegal
CM	Cameroon	LK	Sri Lanka	SU	Soviet Union
DE	Germany	LU	Luxembourg	TD	Chad
DK	Denmark			TC	Togo
				US	United States of America

- 1 -

MODIFIED SEED STORAGE PROTEINS

5        This invention relates to plant seed storage proteins, and in particular to methods of modifying said proteins at specific sites.

Background of the Invention

Over the last few years there has been dramatic  
10 progress in the development of gene transfer systems for  
higher plants, and systems are now available for  
monocotyledonous plants, as well as for a variety of  
dicotyledonous plants. It is now possible not only to  
introduce foreign genes (including non-plant genes) into plant  
15 cells and tissues, and to regenerate whole plants, but also to

control the site in the plant where such genes will be expressed. Methods for introducing genes into plants, and the prospects which these methods offer for applying genetic engineering methods to improvement of crops, have recently 5 been reviewed (C.S. Gasser and R.T. Fraley (1989) *Science* 244 1293-1299); this review reflects the state of the art. International Patent Application No. WO/8903887 discloses a process for production of a mammalian peptide via expression of a modified seed storage protein gene in a transgenic plant. 10 The most commonly used vector is Agrobacterium tumefaciens Ti plasmid, which is successful in transferring genetic information into a variety of dicotyledonous plants, including peas and beans. More recently, the plant virus geminivirus has been proposed as a general purpose vector for use with 15 plants (Australian Patent Application No. 599609 (64380/86) by Monsanto Company and David Bisaro)

Genetic engineering of improved grain crops has been hampered by the lack of detailed structural information about functional storage proteins, which form the major protein 20 component of plant seeds<sup>1</sup>. After synthesis and processing, these proteins are transported to membranous organelles, known as protein bodies, where they accumulate in large amounts<sup>2-4</sup>. Upon germination, they are degraded by endogenous proteases to provide nutrition for the growing plant<sup>5</sup>. Because of the high 25 level of expression and subsequent accumulation of these proteins, they determine the nutritional value of the seed and dictate the requirement for supplements when the seed is used as foodstuff for man or domestic animals.

Most of the protein found in mature seeds belongs to 30 a class called the seed storage proteins. This term is used to describe those proteins whose function is to provide, upon germination, a source of fixed carbon and nitrogen to sustain the early heterotrophic growth of the seedling. However, it is because of the importance of seeds to human nourishment 35 that so much work has been directed at understanding seed proteins. Among the best characterised of the seed proteins

are those from the agriculturally important legumes, soya bean (Glycine max), garden pea (Pisum sativum) and French bean (Phaseolus vulgaris), although increasing attention is being given to food crops of the Third World, including cow pea 5 (Vigna unguiculata), mung bean (V. radiata) and pigeon pea (Cajanus cajan).

As a whole, legume storage proteins, which are mostly of the salt-soluble globulin class, are a nutritionally-poor source of tryptophan and the sulphur-10 containing amino acids, methionine and cysteine, although some of the other protein fractions within the seed (for example the albumins) may have adequate levels of these essential amino acids. Much effort has been directed to improving the understanding of storage proteins so as to be able to 15 manipulate their genes using methods such as recombinant DNA techniques, tissue culture and plant breeding in such a way as to enhance the nutritional value of seed proteins for human and other monogastric animals.

There are two major types of storage proteins in 20 legume seeds, known respectively as vicilins and legumins, which are distinguishable by their sedimentation coefficients (7S/11S), oligomeric organisation (trimeric/hexameric) and polypeptide chain structure (single chain/disulphide linked pair of chains)<sup>6-12</sup>. Both types are found within an 25 individual storage body<sup>13,14</sup>. Analysis of amino-acid sequence data from these two classes suggests that they may be evolutionarily and structurally related<sup>15,16</sup>. Clear sequence relationships have been established within the classes<sup>12</sup>. Furthermore, a sequence motif common to legumins and 30 vicilins<sup>15</sup> has been found to occur twice in vicilins<sup>16</sup>, suggesting a repeated structural motif in vicilins.

Genes encoding two vicilin-type proteins have been isolated from pea (Pisum sativum), and transgenically expressed in tobacco, and their regulatory DNA sequence 35 elements have been identified; these sequences respectively

govern the specificity of expression and level of transcription (Newbigin, E.J. and T.J.V. Higgins: Proc. 8th Australian Biotechnology Conference, Sydney 1989, 104-109)

Attempts have been made to improve the functional properties and nutritional value of glycinin, one of the major storage proteins of soybean, by producing cDNAs encoding glycinins modified by deletion of subsequences and by addition of sequences encoding four continuous methionines. The authors have shown expression and accumulation of some of the 10 mutant proteins in E. coli cells (Kim et al., 1990).

However, their result is inconclusive, at best preliminary, as no attempt is made at expression in plant systems. Furthermore, these authors were limited in that they could only make changes to highly variable regions of the 15 sequence, and then only in an ad hoc fashion. Their methods cannot be generally applied across a spectrum of legumins or vicilins. Indeed, the regions they have modified are regions of low homology to the vicilins, and therefore of no immediate application to vicilins. Nevertheless, their work does 20 underscore that it is realistic to make modified seed storage proteins with improved properties according to the present invention.

Another seed storage protein, arcelin, has been identified in certain wild forms of Phaseolus vulgaris (Romero 25 A. et al (1986) Theor. Appl. Genet. 72 123-128; Osborn et al. (1986) Theor. Appl. Genet. 71 847-855); these proteins are toxic to bruchid pests of beans, and transfer of the cloned arcelin gene to other bean plant confers insect resistance (European Patent Application No. 337750: The Plant Cell 30 Research Institute Inc).

In order to enable us to engineer novel properties into seeds without prejudicing their performance in vivo, we have for the first time determined the three-dimensional structure of phaseolin, the major 7S storage protein from the 35 French Bean Phaseolus vulgaris. With this structural information, we can select suitable sites for modification.

Specific protein engineering targets in this system include improved nutritional value, altered stability with respect to functionality in food systems, and general use as a high-level expression system.

5 Phaseolin, a vicilin-like molecule, is a trimer of three similar glycosylated polypeptides of molecular weights around 50 000<sup>17</sup>. Unlike other vicilins, the phaseolin trimer ( $M_r$  about 150 000) associates into a dodecamer<sup>18</sup> below pH 4.5.

Because of the sequence and structural relationships 10 between vicilins and legumins referred to above and further discussed hereinafter, we consider that phaseolin is a suitable model for legume 7S and 11S storage proteins in particular, and seed storage 7S and 11S proteins in general. Phaseolin has been expressed in transgenic plants<sup>45</sup>.

15 Madison et al. have recently used the three-dimensional structure of the complex between trypsin and bovine pancreatic tissue inhibitor to predict the site of interaction between tissue plasminogen activator (tPA) and plasminogen activator inhibitor-1 (PAI-1). Although the 20 three-dimensional structures of tPA and PAI-1 are not known, tPA and trypsin have sequence similarities. Using these similarities, the authors identified a loop, and one particular residue within the loop, which forms part of the interactive surface between PAI-1 and tPA; by changing the 25 sequence of this loop by site-directed mutagenesis, they produced tPA which was less susceptible to inhibition (E.L. Madison, E.J. Goldsmith, R.D. Gerard, M-J.H. Gething, and J.F. Sambrook (1989) *Nature* 339 721-724).

This strongly suggests that the three-dimensional 30 structure of phaseolin can be used to predict the three-dimensional structures of other vicilins and of legumins.

We have found that the polypeptides of the trimeric seed storage protein phaseolin comprise two 35 structurally-similar units each made up of a  $\beta$ -barrel and an  $\alpha$ -helical domain. The  $\beta$ -barrel has the "jelly-roll" folding

topology shown by viral coat proteins and the  $\alpha$ -helical domain shows structural similarity to the helix-turn-helix motif found in certain DNA-binding proteins. The tetramer of trimers referred to above turns out to be the form of the 5 molecule in the crystals studied here.

Current experience suggests that protein structure is remarkably stable to manipulation by site-directed mutagenesis. Moreover, functional properties of  $\alpha/\beta$  barrel proteins, 8-stranded  $\beta$ -barrel enzymes, and four-helix 10 frameworks are stable to insertions and other modifications (reviewed by D. Ringe (1989) Nature 339 658-9).

#### Summary of the Invention

The major barrier to modifying plants to produce seed storage proteins with commercially desirable properties 15 is knowledge of the three-dimensional structure of the storage proteins.

We have now determined the three-dimensional structure of a representative seed storage protein, phaseolin. Current knowledge in the construction of transgenic plants, 20 and in protein structure and engineering, enables us to use this three-dimensional structure to select target sites in the structure for one or more of the following modifications:

- (a) introduction of point mutations;
- (b) deleting or inserting sequences;
- 25 (c) adding glycosylation sites;
- (d) introducing disulphide bonds.

Thus, based on the three-dimensional structure disclosed herein, and experimental protocols known to persons skilled in the art, the following modifications can be made:

- 30 (i) Introduction of new N-linked glycosylation sites for altering the stability and/or solubility of the protein;
- (ii) Substitution of internal amino acids by methionine to raise the sulphur content of the seed;

(iii) Truncation of protease-susceptible loops on the structure to improve stability;

(iv) Introduction of protease-labile loops to improve the digestive properties;

5 (v) Introduction of disulphide bonds or other stabilising mutations to protect the storage protein structure on passage through the rumen to improve the nutritional value of the protein for ruminants;

10 (vi) Introduction of heterologous protein or peptide sequences into the structure to enable their production in crops; and

(vii) Modifications to the sequence to enhance resistance of the seeds or products thereof to 15 pests such as insects.

Aspects of these properties that are relevant in food systems include:

(a) stability and pH solubility for the large scale extraction of the proteins from seeds;

20 (b) acid solubility for protein enriched beverages;

(c) thermostability for heat-setting properties in snack foods; and

(d) amino acid composition for nutritional 25 balance.

In one aspect, the present invention provides a mutein which is a variant of a naturally-occurring legume seed storage protein, wherein said mutein has a modified primary structure relative to said legume storage protein, but retains 30 the tertiary and quaternary structure of said legume storage protein.

For the purposes of this specification, retention of the tertiary and quaternary structure is to be understood to mean that elements of that tertiary and quaternary structure 35 which are not the subject of primary structure modifications are substantially unaffected by said modifications.

Thus according to one preferred embodiment of the present invention there is provided a plant 7S or 11S storage protein modified at a specific amino acid residue or a specific region of its amino acid sequence, wherein the 5 tertiary and quarternary structure of the naturally occurring storage protein is retained.

Preferably the modification is selected from the group consisting of:

- 10 (a) introduction of one or more point mutations;
- (b) deletion of one or more defined sequences of amino acids;
- (c) insertion of one or more defined sequences of amino acids;
- (d) introduction of one or more glycosylation 15 sites; and
- (e) introduction of one or more disulphide bonds.

More preferably the modification is selected from the group consisting of:

- 20 (a) introduction of N-linked glycosylation sites;
- (b) substitution of internal amino acids by methionine;
- (c) truncation of protease-labile loops; and
- (d) introduction of protease-labile loops.

According to a second aspect of the invention, there 25 is provided a DNA molecule whose sequence encodes a mutein, as defined above. Preferably this DNA encodes a protein having the properties of a plant 7S or 11S storage protein, and also encodes one or more of the modifications set out above.

Plasmids, expression vectors, and microorganisms comprising 30 said DNA are also within the scope of the invention.

According to a third aspect of the invention there is provided a transgenic plant or part thereof having a DNA sequence as defined above.

Preferably the plant part is a seed.

It will be evident to the person skilled in the art that the changes to the seed storage proteins provided by the method according to the invention will have to be made in the first instance at the DNA level. The modified DNA thus 5 represents the initial embodiment of the changes; such DNA will be converted, via the processes of transcription and translation in the cell, to yield the modified seed storage protein.

Brief Description of the Drawings

10 Figure 1 (25 sheets) represents the atomic co-ordinates of phaseolin in orthogonal Å units. The three-fold symmetry axis of the phaseolin trimer is coincident with the Y axis of the co-ordinate frame. The coordinates of the C atoms have been deposited by the applicant in the 15 Brookhaven Protein Data Bank.

Figure 2 represents schematic diagrams showing the two observed patterns of interaction between the  $\alpha+\beta$  structural units. The absence of residues 213-219 in the electron density map leaves an ambiguity as to which is the 20 correct pairing of the  $\alpha+\beta$  units to form the polypeptide. (a) represents the preferred polypeptide (see text). In both diagrams the view is down the molecular three-fold axis and from the centre of the tetramer outwards. The pseudo-diads relating the structural units lie in the plane of the paper, 25 intersecting the molecular three-fold.

Figure 3 represents a stereo pair showing a  $C\alpha$  trace of the phaseolin trimer, viewed down the molecular three-fold towards the centre of the tetramer. The N- and C-termini of each subunit are labelled. The two possible ways 30 of linking the two  $\alpha+\beta$  units to form the subunit are indicated: the shorter link of 17Å (solid line) is favoured above the longer 34Å link (dashed line). The figure was drawn using a computer program written by Lesk and Hardman<sup>31</sup>.

Figure 4 is a diagram showing the structure of native phaseolin (A) and the proposed high-methionine mutant phaseolin (B) in the neighbourhood of residues 84 to 88. The methionine sidechains of the mutant are seen to be 5 accommodated in the structure without disruption to the tertiary or quaternary structure of the protein. For clarity, residues in the same  $\beta$ -sheet as residues 84 to 88 are not shown.

Figure 5 is a diagram showing the structure of 10 native phaseolin (A) and the proposed high-methionine mutant phaseolin (B) in the neighbourhood of residues 261-265. The methionine sidechains of the mutant are seen to be 15 accommodated in the structure without disruption to the tertiary and quaternary structure of the protein. For clarity, residues in the same  $\beta$ -sheet as residues 261-265 are not shown.

#### Structure Description

X-ray diffraction data to 3 $\text{\AA}$  resolution were collected from Type II crystals of phaseolin<sup>19</sup> and heavy atom 20 derivatives. The methods of analysis do not form part of this invention. However, various attempts to solve the structure by multiple isomorphous replacement and non-crystallographic symmetry averaging were unsuccessful over a period of 6 years, until a cautious approach using phase extension procedures was 25 adopted.

#### Structural heterogeneity

Three different genes encoding potential protein products have been identified by gene sequencing<sup>11</sup>. These differ only in number of amino acids, and contain 397, 411 and 30 412 amino acids respectively, after allowing for cleavage of a 24 amino-acid signal sequence. The sequence and numbering used here is given in Table 1.

---

1	TSLREEEE	SDNPFY	FNSD	NSWNTLF	KNQYGH	IRVLQR	FDDQ	QSKRLQ	NLEDY	YRLVE	FRSK	B
	[ V ]	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	60
61	PETL	LLPQQ	A	DAELL	LLV	RSGS	A	ILVL	V	KPDDR	REYFF	LTSDNPI
	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....
121	VNRDP	KEDL	R	I	QI	LAMP	VNN	PQI	HEFF	LSSTE	AQQSYL	QEF
	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....
181	LFEEEG	QQEG	VIV	NID	SEQI	KELSKH	A	AKSS	RKSLSK	QDNTIG	NEFGN	LERTD
	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....
241	ISSIEMEE	EGALF	VPH	Y	SKAI	VIL	VV	NEGEA	HVELV	GPKGN	KETLEY	YESYRAE
	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....
301	VIPAA	YPV	AIKAT	SVN	FTG	GIN	NNNN	RNLL	AGKT	DNV	ISSIGR	ALDGKDVL
	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....
361	SGDEV	MKLINK	QSGSY	FVDAHH	HQQE	QQKGR	KGAF	VY				
	.....	.....	.....	.....	.....	.....	.....	.....				

---

Table 1. Amino-acid sequence of the shorter (397 residue)  $\beta$ -type phaseolin polypeptide. The line underneath the sequence contains the following symbols.  $\alpha$ : regions of  $\alpha$ -helical secondary structure,  $\beta$ : regions of  $\beta$ -sheet secondary structure, G: glycosylation sites, [ ]: regions of unobserved electron density, I: intron locations, V: points of major sequence insertion in other vicilin proteins. Shown above the sequence are the labels used to denote the secondary-structural elements in the text. Note that the secondary structure assignments are based on the current unrefined model and thus that the precise start and end points of the strands and helices may be in error by one or two amino acids in some places.

Compared with the 397 residue protein, the 411 residue protein has a five amino-acid insertion after residue 189 and a nine amino-acid insertion after residue 390. The 412 residue protein has a further insertion of one amino acid 5 after residue 100. The chain trace of the electron density map (not shown) is that of the 397 amino-acid protein (termed the  $\beta$ -type polypeptide<sup>11</sup>) and shows no break or weakening of electron density in the vicinity of residue 189. We thus conclude that the 397 amino-acid protein is overwhelmingly 10 dominant in the crystal. It will be clear to the person skilled in the art that these three genes can be readily interconverted, using presently available techniques. This invention is to be understood to apply to all three forms of the protein.

15 The map shows weak evidence of glycan binding at both known Asn-X-Ser/Thr glycosylation triplets<sup>24</sup>. The density is not yet sufficiently clear to provide information about the nature of heterogeneity of the glycans.

#### Folding topology

20 Figure 2 shows a schematic drawing of the polypeptide. It consists of two structurally-similar units of about 160 amino acids each. These are related by a pseudo-diad axis nearly perpendicular to and intersecting the molecular triad axis. Each unit is itself an  $\alpha + \beta$  two-domain 25 structure, the first of some 110 residues being a classic viral capsid jelly-roll structure, and the second smaller domain being a cluster of three helices, including a helix-turn-helix motif. A fourth helix in the N-terminal unit, which is not structurally

associated with the three-helix cluster, forms part of the connection through to the C-terminal unit.

The jelly-roll barrel structure in phaseolin is stripped of nearly all of the elaboration seen in the viral capsid proteins<sup>25,26</sup>; in this respect it is similar to the barrel structure observed in catabolite gene activator protein (CAP)<sup>27</sup>. It is convenient to denote the eight strands of the jelly-roll  $\beta$ -barrel as B through I, in analogy with the notation used in the discussion of the viral capsid proteins<sup>25</sup>. In only two places in phaseolin is there found a loop of structure external to the barrel, between strands F and G of the N-terminal barrel (residues ca 102-108) and between strands E and F of the C-terminal barrel (residues ca 277-286). Each barrel has an A strand reminiscent of the C subunits of the plant virus capsid proteins<sup>25</sup>, and another  $\beta$ -strand, antiparallel and N-terminal to A, which we label here strand A'. Both barrels have a further strand (which we label J) C-terminal to the barrel, making a total of eleven strands in the  $\beta$ -sheet structure. Strands C of each barrel have a bulge at positions 65-68 and 252-255 respectively.

The helical domains comprise residues ca 156-181 and 340-371, each being a three-helix cluster. These helices bear a striking similarity to a helix-turn-helix motif in Cro, a DNA binding protein<sup>28</sup>. This will be discussed further below. The occurrence on a single polypeptide of a jelly-roll  $\beta$ -barrel and a helical cluster reminiscent of DNA binding proteins has previously been observed for the CAP protein. However, the

relative position of these two domains in phaseolin and CAP is very different.

The internal sequence repeat<sup>16</sup> observed in phaseolin, jack bean canavalin and pea vicilin is the basis for the structural repeat described here. The sequence similarity in the internal repeat is low ( $\approx 15\%$  identity), but the amino-acid alignment corresponds to the structural repeat perfectly in many places and to within a few residues in the worst cases. The domains are remarkably similar; a least-squares fit of the  $\text{C}\alpha$  positions in corresponding structural elements of the pair of units yields an r.m.s. deviation of only 2.2 $\text{\AA}$ .

Exon/intron boundaries are the same in phaseolin and conglycinin DNA sequences<sup>29,7,12</sup>. Those five boundaries are, in the first unit, at the DE corner (residue 81), within the J  $\beta$ -strand (144), the H2-H3 corner (171); and in the second unit, the BC corner (248) and the  $\beta$ - $\rightarrow$  $\alpha$  connection (335). If strand J is considered as a linking element between the  $\beta$  and  $\alpha$  structures, then all these boundaries lie at the interconnection of various elements of the secondary structure.

#### Trimer structure

The six structural  $\alpha+\beta$  units which comprise the phaseolin trimer are arranged alternately up and down around the three-fold axis and are nearly coplanar. The trimer is therefore a disc of diameter 90 $\text{\AA}$  and thickness 35 $\text{\AA}$ , as predicted by electron microscopy<sup>30</sup> and exhibits approximate 32

point group symmetry. Such an arrangement suggests two types of 'interfaces' between the units, intrachain contacts within one polypeptide, and trimer contacts between the three chains. Each interface is centred around a pseudo-diad relating the two structurally-similar units of the polypeptide. No electron density is visible for the region linking the units ( residues 213-219) leaving an apparent ambiguity as to which adjacent pair of units in the trimer is on the one polypeptide chain (see Figure 3). One pair has a distance of 37Å between the  $\text{C}\alpha$  positions of residues 212 and 220, and the other has a corresponding distance of 18Å. To avoid postulating an extremely extended polypeptide linker, we conclude tentatively that the subunit is most likely formed from the latter pair. (The question of definition of the trimer within the tetramer will be discussed below; for completeness it should be pointed out that it is not possible for the missing polypeptide link to run from an N-terminal unit in one trimer to the C-terminal unit in another as these are separated by  $\approx 60\text{\AA}$ ).

The jelly-roll  $\beta$ -barrel has a remarkable capacity to exist in different states of oligomerization<sup>32,33</sup>. The hexameric pattern observed here with quasi-32 point group symmetry is unlike the packing around the quasi-6-fold axis of the T=3 icosahedral surface lattice<sup>26</sup>. Furthermore the specific interactions between the barrels seen here are unlike those observed in T=1 capsids<sup>25</sup>, tumour necrosis factor<sup>34</sup> or in the adenovirus hexon<sup>33</sup>.

The B-I-D-G face of the two barrels associate with each around

the pseudo-diad in what appears to be a typical example of aligned packing of  $\beta$ -sheets. The two potential N-linked glycosylation sites are both within the C-terminal barrel on strands A and I respectively. The sugar attached to strand I could contact the neighbouring N-terminal barrel.

The helical domains of the subunits are closely associated with each other around the pseudo-diad relating the neighbouring subunits (see Figure 2b). As mentioned above, the helix-turn-helix motifs formed by helices 2 and 3 of each domain are similar to those found in certain DNA-binding proteins<sup>35</sup>, typified by the Cro protein. A least-squares fit of the C $\alpha$  positions of residues 163-183 and 351-371 of phaseolin to the helix-turn-helix motif formed by residues 16-36 of Cro yields an r.m.s. deviation of 1.9 $\text{\AA}$  and 1.3 $\text{\AA}$  respectively, within the spread determined for these motifs<sup>35</sup>. The capacity of helix-turn-helix structures to bind DNA is associated with their condensation into dimers with diad symmetry coincident with that of double-stranded DNA, in particular with elements of the diad-related helices positioned 34 $\text{\AA}$  apart and binding to consecutive major grooves of DNA. No such 34 $\text{\AA}$  period is evident in the dimerisation of the phaseolin helical domains, nor indeed are the two domains identical. The dimensions of that domain pair are more of the order of 18 $\text{\AA}$  (in the trimer, not the polypeptide as we have chosen to define it here, Figure 3), sufficient only to span adjacent major and minor grooves of DNA. All of the DNA-protein structures solved to date which have helix-turn-helix motifs for the DNA binding site exemplify the diad-symmetrical form of binding.

- 17 -

Recent studies<sup>35,36</sup> of structures in the protein data bank<sup>37</sup> have demonstrated that DNA binding protein II<sup>38</sup>, the ribosomal L7/L12 protein<sup>39</sup> and cytochrome C peroxidase<sup>40</sup> all contain helix-turn-helix motifs. The first two of these bind nucleic acids, whether or not via the helix-turn-helix motif is unknown. However the cytochrome C peroxidase structure embodies the motif semi-internally, making interaction with DNA very unlikely<sup>35</sup>.

In phaseolin the second helix in the motif (i.e. the third in the helical domain) is exposed to the environment in both structural units on the polypeptide and within the trimer (Figure 3). We know of no evidence suggesting that phaseolin is able to bind DNA, specifically or non-specifically. The translocation of the phaseolin polypeptide from its site of synthesis on membrane-bound polysomes through the endoplasmic reticulum into storage bodies<sup>41,3</sup> makes such an interaction unlikely. Nevertheless, DNA-binding studies could provide direct evidence for or against a role for storage proteins in the regulation of their own high level of synthesis.

#### Ligand binding sites

We have previously reported<sup>19</sup> the results of a phosphorus analysis of type II phaseolin crystals which implies that two molecules of phytic acid might be associated with each 50kDa polypeptide. There is no electron-dense feature in the current 3Å map consistent with such binding, though phytate binding to

the flexible ends or linker region of the polypeptide cannot be excluded.

At the interface between the two jelly-roll domains of the subunit involving the sheets B-I-D-G referred to above, there is an intense spherical electron-dense feature lying in a pocket formed by the side chains of residues His 32, Glu 56, Arg 58, Arg 79, Arg 130, Lys 296 and Asp 297. A possible explanation is that it corresponds to phosphate bound either *in vivo* or during the purification process. A second unexplained, though more diffuse, electron-dense feature occurs within the N-terminal  $\beta$ -barrel and is associated with the side chains of residues Gln 133 and Glu 145.

#### **The tetramer of trimers**

The crystallization conditions used here for phaseolin have encouraged the formation of tetrameric 18S particles. The association of trimers into dodecamers under conditions of acid pH is well-characterized<sup>18</sup>, and 18S particles so produced have been imaged by electron microscopy<sup>30</sup>. The 18S particle observed in the crystal, being formed by four trimers assembled on the faces of a regular tetrahedron, is consistent with the negatively stained e.m. image as judged by the positioning of the solvent channels.

There are two ways of grouping the twelve subunit polypeptide chains in the tetrahedron into trimers. Inspection of the particle shows that in the one association, the intra-trimer

polypeptide contacts are extensive (see Figure 3) whereas in the alternate association the subunits are tenuously packed (reminiscent of protein crystal packing). We conclude that the former arrangement is the 7S (150kDa) particle occurring *in vivo* and observed as a featureless disc by electron microscopy<sup>30</sup>, and have used this definition of the trimer in the discussion of the preceding sections. The inter-trimer contact in the tetramer occurs at the tetrahedral diad axes. It consists of a symmetry-related pair of interactions, each involving the N-terminal  $\beta$ -barrel of one subunit with the C-terminal  $\beta$ -barrel of a subunit from the neighbouring trimer. The N-terminal strands of polypeptides from neighbouring trimers are also in contact at the tetrahedral diad.

#### ***In situ* organization**

Although no crystallinity of *Phaseolus vulgaris* seed sections is observable by X-ray diffraction<sup>19</sup>, we cannot rule out a possible link between the curious packing of phaseolin in pseudo-cubic high-salt crystals<sup>19,42</sup> with structures *in situ* in the seed-storage protein body. (Such a link has been demonstrated for the 11S protein cucurbitin<sup>43</sup>). The high-salt crystals, with pseudo-cubic symmetry P432 and cell dimension  $a \approx 66\text{\AA}$ , can contain only one phaseolin trimer per unit cell. What combination of crystal twinning and/or disorder generates the pseudo-cubic point group is unclear. One possibility emerges from the dodecamer structure observed here. The centre-to-centre distance between the trimers in the tetrahedral 18S particle is  $\approx 65\text{\AA}$ . Packing errors, whereby

trimers are incorporated into the tetrahedral structures without proper cognizance of the top and bottom face of the trimer, could lead to non-closed forms of the tetramer (of trimers) and an average structure in which the 65Å period was associated with a cubic point group. Other explanations include the possibility that the pseudo 32 point group of the trimer is not maintained in high salt, but is distorted into a quasi-cubic structure.

#### Related Structures

##### Homology with other vicilins

Sequence alignments imply structural similarity of 7S proteins from common bean, jack bean, soybean and pea seeds<sup>12,15,16</sup>. Insertions and deletions in these alignments are, with minor modifications, compatible with the phaseolin structure (see Table 1). For the most part, the phaseolin sequence is shorter than the other sequences, the exception being a five residue insertion around position 350, which may affect the structure of the connection between helices 1 and 2 of the C-terminal structural unit. Significant insertions in the other sequences are found near the N-terminus and at the FG corner (residue 107, Table 1) of the first barrel domain ( $\alpha'$ -subunit of  $\beta$ -conglycinin of soybean), in the linker between helices 3 and 4 (residue 188) of the first helical domain (pea vicilin), in the linker (residue 218) between the two  $\alpha+\beta$  units (all sequences except phaseolin), and at the EF corner (residue 283) of the second barrel domain (larger inserts for pea proteins

than for soybean). All of these regions are on the surface of the trimer. (The insertion site at residue 218<sup>15</sup> has been placed alternatively at residue 247<sup>12</sup>; we consider that the former leads to the more natural sequence alignment).

A preliminary structure for jack bean canavalin (A. McPherson, personal communication) shows pseudo 32 point group symmetry and a viral capsid domain in each of the two structural units per polypeptide.

#### **Homology with legumins**

Based on amino-acid sequence similarity, the basic polypeptide chain of legumins is believed to contain one copy of the repeating structural unit of a vicilin molecule<sup>16</sup>, i.e. the  $\alpha+\beta$  structure described here. Weak similarity between parts of the acidic chain and the 7S proteins has also been reported, but is less convincing<sup>15</sup>. X-ray diffraction experiments<sup>43</sup> have indicated that the legumin protein cucurbitin has point group symmetry 23, at least at low resolution (ca 20Å). This observation requires that the polypeptide displays an internal repeating structure, which in the 11S particle is a diad, albeit not perpendicular to any three-fold axis. The assembly of the six polypeptides of legumin into the accumulated oligomeric form is believed to proceed via a 7S (trimer) intermediate, the final coalescing of trimers not occurring until cleavage of the polypeptides into the basic and acidic chains<sup>44</sup>. If the trimer form is indeed similar to the vicilin 7S molecules, with pseudo point group 32, then a rearrangement

of the subunits within the trimer must accompany the formation of the 11S particle, in order to satisfy the resulting cubic arrangement of diads and triads.

#### Novel phaseolins

5 One attempt has previously been made to increase the sulphur content of phaseolin by the insertion of a 45 base-pair synthetic duplex, rich in methionine-codons, at the Xba I site<sup>7</sup> in the third exon of the  $\alpha$ -phaseolin gene. Transgenic tobacco plants containing normal or modified 10 phaseolin genes were then monitored for the production and deposition of phaseolin. Whereas in both cases phaseolin expression was achieved, deposition of the modified protein in the storage bodies did not occur, suggesting prior degradation<sup>45</sup>. Using the three-dimensional structure, we are 15 now able to identify the Xba I site (after residue 165, Table 1) as being internal to helix 2 (i.e. the first helix in the helix-turn-helix motif) and hence part of a major structural element of the phaseolin trimer. We therefore predict that an inclusion of fifteen residues at this site could distort the 20 structure at the tertiary and/or quaternary level, making the modified protein more susceptible to degradation.

#### Conclusions

We have now confirmed the internal repeat observed in the sequence of phaseolin at a structural level; this 25 repeat manifests itself as a pair of  $\alpha+\beta$  units forming the 50kDa subunit. The high sequence similarity to other 7S storage proteins suggests a common structure; indeed a preliminary X-ray structure for canavalin, the 7S protein of the jack bean, indicates a hexameric arrangement of  $\beta$ -barrels 30 as described here (A. McPherson, personal communication).

The structure presented here identifies surface regions of the molecule, which represent candidate sites for genetically-engineered insertions into the sequence.

The invention will now be illustrated by way of reference only to the following non-limiting examples. The references to amino acid sequence numbering are as in Table 1.

In these examples, site directed mutagenesis is used 5 to introduce desired mutations at defined sites in known fragments of wild type phaseolin cDNA.

Mutations are introduced by known methods, such as those described by Kunkel (46), into restriction fragments which include the segment of DNA encoding the locus for the 10 desired mutation. The resulting DNA is used to transfect a host, such as E.coli, and single stranded DNA prepared from plaques. The presence of the desired mutation is confirmed by complete sequencing of the same restriction fragment, for example using the method of Sanger et al. (47). The double 15 stranded replicative form of DNAs of proven mutants is isolated, and the mutant restriction fragments isolated by agarose electrophoresis (48). These fragments are then used to replace the corresponding fragment of wild type DNA in an expression vector. All the recombinant methods used are as 20 described by Sambrook et al. (48). Other suitable methods for these procedures would readily occur to the person skilled in the art.

Example 1 - Engineering of High Methionine Phaseolin Mutations

The two sequences selected as targets for 25 engineering of high-methionine phaseolins are "ILVLV" in region E between amino acids 61 and 120, Table 1 and "IVILV" in region D between amino acids 241 and 300, Table 1, which both correspond to hydrophobic domains, ie. regions of internal  $\beta$  structure. Each of these sequences is mutated to 30 code for methionine pockets (MMMMM) by iterated cycles of oligonucleotide site-directed mutagenesis. An intron-less  $\beta$ -phaseolin minigene is mutated; this minigene, designated  $\beta$ wt*i*<sup>-</sup>, has recently been shown to direct efficient expression of phaseolin protein in transgenic tobacco seeds (Bustos et 35 al., 1990; (49)). The advantages of using the minigene

instead of phaseolin genomic DNA fragments derive from the absence of intervening sequences. This facilitates the design of gene constructions and permutations of DNA fragments to combine different mutations. Due to the large number of 5 individual nucleotides that need to be mutated over a span of 15 or 18 nucleotides, a strategy involving multiple rounds of mutagenesis is preferable to one that would attempt to produce all changes at once. This has the added advantage of generating intermediates with fewer than five new methionines, 10 which may be useful when assessing the effects of individual amino acid changes on the structure and in vivo stability of the protein. The detailed mutagenesis strategies are as follows:

"ILVLV" site:

15 A 381 bp EcoRI-PstI restriction fragment from clone  $\beta$ wt<sup>i-</sup> (Bustos et al., 1990) is subcloned into the phagemid vector pBSKS+ (Stratagene) and the resulting clone is used to produce a U-containing single stranded DNA template. Three different synthetic single-stranded oligonucleotide DNA 20 molecules (shown below as oligos I to III) are utilized to mutagenize the wt sequence by the method of Kunkel (46). The individual base substitutions are indicated in boldface. Screening of mutated clones is performed directly by sequencing with an oligonucleotide primer designed to 25 hybridize 35 nucleotides upstream of the target sequences.

		<sup>81</sup> gly ser ala <u>Ile Leu Val Leu Val</u> lys pro asp <sup>91</sup>
wt	...	ggg agc gcc ATA CTC GTC TTG GTG aaa cct gat ...
oligo I		5' agc gcc ATG ATG GTC TTG <sup>3'</sup>
oligo II		5' G GTC TTG ATG aaa cct <sup>3'</sup>
30 oligo III		5' gcc ATG ATG ATG ATG aaa cct <sup>3'</sup>
final	<sup>81</sup> gly ser ala <u>Met Met Met Met Met</u> lys pro asp <sup>91</sup>	...
		... ggg agc gcc ATG ATG ATG ATG AAA CCT GAT ...

After each round of mutagenesis has been completed, the new EcoRI-PstI DNA fragments are replaced into the  $\beta$ wt<sup>i-</sup> gene to yield modified phaseolin genes coding for two, three and five new methionine residues.

5 "IVILV" site"

A 2.0 kbp XbaI-BamHI restriction fragment from clone  $\beta$ wt<sup>i-</sup> (Bustos et al., 1990) is subcloned into the phagemid vector pBSKS+ (Stratagene) and the resulting clone used to produce a U-containing single-stranded DNA template. In a manner analogous to that employed at the ILVLV site, three synthetic oligonucleotides (oligos IV to VI, shown below) are used to mutagenize the wt sequence using the same method. As for the other site, each oligo is designed to mutate two or three closely spaced nucleotides, and all oligos result in at least one new methionine codon.

	258	ser lys ala <u>Ile Val Ile Leu Val</u> val asn glu gly <sup>269</sup>
wt	...	tct aag gcc ATT GTT ATA CTA GTG gtt aat gaa gga ..
oligo IV	5'	aag gcc ATG ATG ATA CTA GT <sup>3'</sup>
oligo V	5'	TG ATA CTG ATG gtt aat <sup>3'</sup>
20 oligo VI	5'	TG ATG ATG ATG ATG gtt <sup>31</sup>
final	258	ser lys ala <u>Met Met Met Met Met</u> val asn glu gly <sup>269</sup>
	...	tct aag gcc ATG ATG ATG ATG ATG gtt aat gaa gga ..

As for the ILVLV site, the sequences at and around the mutated sites are verified using a sequencing primer that hybridizes near the site. After mutagenesis the XbaI-BamHI fragments are replaced into  $\beta$ wt<sup>i-</sup> or into the high-methionine mutants modified at the ILVLV site. A maximum of ten new methionine residues result from the combination of mutations at both sites.

30 All mutated phaseolin genes are subsequently subcloned into the binary vector pBIN19 and transferred into the genome of tobacco by A. tumefaciens-mediated transformation.

Example 2 - Model Building of High-Methionine Mutant Phaseolin

The structure of the high-methionine mutant phaseolin can be investigated by model-building as follows. An interactive molecular-graphics computer program (QUANTA, 5 Polygen Corporation) was used to model the replacement of residues 84 to 88 and 261 to 265 by methionine. The energy-refinement computer-program XPLOR (Harvard University) was then used to refine the atomic coordinates of the mutant structure to ensure that favourable stereochemistry is 10 achieved, keeping the remainder of the protein as close as possible to the native structure. The results of the modelling are shown in Figures 4 and 5; there are no significant difference in energy between the native and mutant structures (native: -11529 Kcal/mol, mutant: -11677 Kcal/mol) 15 and no disruption to the tertiary or quaternary structure is predicted.

Example 3

The environment of the following residues in the phaseolin structure indicates that they can be altered to 20 Methionine without prejudice to the three-dimensional structure of the protein:

Leu 65, Leu 76, Phe 252, Leu 264, Ile 177, Leu 181.

Example 4

Mutation of Isoleucine 105 to Asparagine introduces 25 an N-linked glycosylation site at that position. Sugar attached at that site may be accommodated on the surface of the phaseolin trimer.

Example 5

Elimination of the loop of structure between beta 30 strands E and F of the C-terminal structural unit may be accomplished by deleting residues numbered 278 to 287 and

replacing them with a linker of two glycine residues. This increases the stability of phaseolin to enzymes with trypsin-like specificity.

In general, the selection of sites for mutagenesis 5 may be influenced by the accessibility of the target site to restriction endonucleases. The criteria for assessing whether the desired mutation has been achieved will depend on the nature of the mutation attempted, but include;

- 10 a) sequencing of the DNA in the construct;
- b) analysis of the product protein for presence or absence of the desired property, eg. by amino acid analysis or susceptibility to enzymes;
- c) retention of tertiary or quaternary structure;
- d) cross-reaction with antibody directed against 15 the native protein; and
- e) successful expression in vivo.

For example, if the mutation is to substitute methionine for another amino acid, the presence of one or two met residues could be detected by cyanogen bromide cleavage; 20 the presence of about 10 met residues could be readily assayed by amino acid analysis. Retention of three dimensional structure (tertiary or quaternary) can be assessed in advance by model building, and tested in the protein actually produced by success in expression in vivo, and by various physical 25 analyses such as molecular weight, solubility, and circular dichroism spectral studies. Other suitable methods will be known to those skilled in the art.

Although the invention has been illustrated with reference to phaseolin, sequence homologies indicate that 30 similar results may be expected with related proteins, such as the homologous protein from pea, and to some extent with legumins as implied by the homology described in reference 16.

References cited herein are identified in full on the following pages.

It will be clearly understood that the invention in its general aspects is not limited to the specific details referred to hereinabove.

References

1. Derbyshire, E., Wright, D.J. & Boulter, D. *Phytochem.* **15**, 3-24 (1976).
2. Varner, J.E. & Schidlovsky, G. *Plant Physiol. (Bethesda)* **38**, 139-144 (1963).
3. Bollini, R., Van der Wilden, W. & Chrispeels, M.J. *Physiol. Plant* **55**, 82-92 (1982).
4. Bollini, R., Vitale, A. & Chrispeels, M.J. *J. Cell. Biol.* **96**, 999-1007 (1983).
5. Millerd, A. *Ann. Rev. Plant Physiol.* **26**, 53-72 (1975).
6. Croy, R.R.D., Lycett, G.W., Gatehouse, J.A., Yarwood, J.N. & Boulter, D. *Nature* **295**, 76-79 (1982).
7. Slightom, J.L., Sun, S.M. & Hall, T.C. *Proc. Natl. Acad. Sci. USA* **80**, 1897-1901 (1983).
8. Marco, Y.A., Thanh, V.H., Tumer, N.E., Scallon, B.J. & Nielsen, N.C. *J. Biol. Chem.* **259**, 13436-13441 (1984).
9. Hirano, H., Fukazawa, C. & Harada, K. *J. Biol. Chem.* **259**, 14371-14377 (1984).
10. Higgins, T.J.V. *Ann. Rev. Plant Physiol.* **35**, 191-221 (1984).

11. Slightom, J.L., Drong, R.F., Klassy, R.C. & Hoffman, L.M. *Nuc. Acids Res.* 13, 6483-6498 (1985).
12. Doyle, J.J., Schuler, M.A., Godette, W.D., Zenger, V., Beachy, R.N. & Slightom, J.L. *J. Biol. Chem.* 261, 9228-9238 (1986).
13. Graham, T.A. & Gunning, B.E.S. *Nature* 228, 81-82 (1970).
14. Craig, S., Millerd, A. & Goodchild, D.J. *Aust. J. Plant Physiol.* 7, 339-351 (1980).
15. Argos, P., Narayana, S.V.L. & Nielsen, N.C. *EMBO J.* 4, 1111-1117 (1985).
16. Gibbs, P.E.M., Strongin, K.B. & McPherson A., *Mol Biol. Evol.* 6, 614-623 (1989).
17. Ma, Y., Bliss, F.A. & Hall, T.C. *Plant Physiol.* 59, 1122-1124 (1977).
18. Sun, S.M., McLeester, R.C., Bliss, F.A. & Hall T.C. *J. Biol. Chem.*, 249, 2118-2121 (1974).
19. Suzuki, E., Van Donkelaar, A., Varghese, J.N., Lilley, G.G., Blagrove, R.J. & Colman, P.M. *J. Biol. Chem.* 258, 2634-2636 (1983).
20. Rossman, M.G. & Blow, D.M. *Acta Cryst.* 15, 24-31 (1962).
21. Wang, B.C. *Meth. Enzym.* 115, 90-112 (1985).

22. Rayment,I. *Acta Crystallogr. A39*, 102-116 (1983).
23. Jones,T.A. *J.Appl.Cryst. 11*, 268-272 (1978).
24. Sturm,A., Van Kuik,J.A., Vliegenthart,J.F.G. & Chrispeels,M.J. *J.Biol.Chem. 262*, 13392-13403 (1987).
25. Rossman,M.G., Abad-Zaperto,C., Murthy,M.R.N., Liljas,L, Jones,T.A. & Strandberg,B. *J.Mol.Biol. 165*, 711-736 (1983).
26. Rossman,M.G. *BioEssays 7*, 99-103 (1987).
27. McKay,D.B., Weber,I.T. & Steitz,T.A. *J. Biol. Chem 257*, 9518-9524 (1982).
28. Anderson,W.F. Ohlendorf,D.H., Takeda,Y. & Matthews,B.W. *Nature 290*, 754-758 (1981).
29. Sun,S.M., Slightom,J.L. & Hall,T.C. *Nature 289*, 37-41 (1981).
30. Tulloch,P.A. & Blagrove,R.J. *Arch. Biochem. Biophys. 241*, 521-532 (1985).
31. Lesk,A.M. and Hardman,K.D. *Science 216*, 539-540 (1982).
32. Argos,P., Tsukihara,T. & Rossman,M.G. *J.Molec.Evol. 15*, 169-179 (1980).

33. Roberts, M.M., White, J.L., Grütter, M.G. & Burnett, R.M. *Science* 232, 1148-1151 (1986).

34. Jones, E.Y., Stuart, D.I. & Walker, N.P.C. *Nature* 338, 225-228 (1989).

35. Brennan, R.G. & Matthews, B.W. *J.Biol.Chem.* 264, 1903-1906 (1989).

36. Richardson, J.S. & Richardson, D.C. *Proteins:Structure, Functions and Genetics* 4, 229-239 (1988).

37. Bernstein, F.C., Koetzle, T.F., Williams, G.J.B., Meyer, E.F., Brice, M.D., Rodgers, J.R., Kennard, O., Shimanouchi, T. & Tasumi, M. *J.Mol.Biol.* 112, 535-542 (1977).

38. Tanaka, I., Appelt, K., Dijk, J., White, S.W. & Wilson, K.S. *Nature* 310, 376-381 (1984).

39. Leijonmarck, M., Eriksson, S. & Liljas, A. *Nature* 286, 824-826 (1980).

40. Poulos, T.L., Freer, S.T., Alden, R.A., Edwards, S.L., Skoglund, U., Takio, K., Eriksson, B., Xuong, N.H., Yonetani, T. & Kraut, J. *J.Biol.Chem.* 255, 575-580 (1980).

41. Baumgartner, B., Tokuyasu, K.T. & Chrispeels, M.J. *Planta (Berl.)* 150, 419-425 (1980).

42. Johnson, S., Grayson, G., Robinson, L., Chahade, R., & McPherson, A., *Biochemistry* 21, 4839-4843 (1982).
43. Colman, P.M., Suzuki, E., & Van Donkelaar, A., *Eur. J. Biochem.* 103, 585-588 (1980).
44. Dickinson, C.D., Floener, L.A., Lilley, G.G., & Nielsen, N.C., *Proc. Natl. Acad. Sci. USA* 84, 5525-5529 (1987).
45. Hoffman, L.M., Donaldson, D.D., & Herman, E.M., *Plant Mol. Biol.* 11, 717-729 (1988).
46. Kunkel, T., *Proc. Nat. Acad. Sci. USA* 82 488-492 (1985).
47. Sanger, F., Nicklen, S., and Coulson, A.R., *Proc. Nat. Acad. Sci. USA* 74 5463-5467 (1972).
48. Sambrook, J., Fritsch, E., and Maniatis, T. *Molecular Cloning: A Laboratory Manual* 2nd ed. (Cold Spring Harbor Press, 1989).
49. Bustos, M.M., Kalkan, F.A., VandenBosch, K.A. and Hall T.C., *Plant Mol. Biol.*, Submitted.

CLAIMS:

1. A mutein which is a variant of a naturally-occurring legume seed storage protein, wherein said mutein has a modified primary structure relative to said legume storage protein, but retains the tertiary and quaternary structure of said legume storage protein.
2. A plant 7S or 11S storage protein modified at a specific amino acid residue or a specific region of its amino acid sequence, wherein the tertiary and quaternary structure of the naturally occurring storage protein is retained.
3. A storage protein according to Claim 1 or Claim 2, wherein the modification is selected from the group consisting of:
  - (a) introduction of one or more point mutations;
  - (b) deletion of one or more defined sequences of amino acids;
  - (c) insertion of one or more defined sequences of amino acids;
  - (d) introduction of one or more glycosylation sites; and
  - (e) introduction of one or more disulphide bonds.
4. A plant storage protein according to Claim 3, wherein the modification is selected from the group consisting of:
  - (a) introduction of N-linked glycosylation sites;
  - (b) substitution of internal amino acids by methionine;
  - (c) truncation of protease-labile loops; and
  - (d) introduction of protease-labile loops.
5. A protein according to any one of Claims 1 to 5 which is a vicilin or a legumin.
6. A protein according to Claim 5 which is a phaseolin.
7. A DNA molecule whose sequence encodes a storage protein as defined in any one of Claims 1 to 6.

8. A DNA molecule according to Claim 7, whose sequence encodes a protein having the properties of a plant 7S or 11S storage protein, and also encodes one or more of the modifications set out above.
9. A DNA molecule according to Claim 8 wherein the protein is a vicilin or a legumin.
10. A DNA molecule according to Claim 9 wherein the protein is phaseolin.
11. An autonomous unit of DNA replication in vivo or in vitro selected from the group consisting of plasmids, cosmids, expression vectors, microorganisms, viruses and chromosomes, said autonomous unit comprising a DNA molecule according to any one of Claims 7 to 10.
12. A autonomous unit of DNA replication according to Claim 11 which is Agrobacterium tumefaciens.
13. A autonomous unit of DNA replication according to Claim 11 which is a plant virus.
14. A transgenic plant or part thereof comprising a DNA sequence as defined in any one of Claims 7 to 10.
15. A seed of a transgenic plant according to Claim 14.
16. A product obtained from a plant according to Claim 14.

1/32

III . 1.1

ASP CB	11	2.38	-16.30	22.82	:	ASP CG	11	3.50	3.50	23.77
ASP OD1	11	3.32	-16.13	24.98	:	ASP OD2	11	4.54	4.54	23.28
ASP C	11	3.49	-18.33	21.93	:	ASP O	11	4.63	4.63	21.67
ASP N	11	2.22	-16.70	20.49	:	ASP CA	11	3.07	3.07	21.63
ASN N	12	2.64	-19.23	22.45	:	ASN CA	12	2.97	2.97	22.44
ASN CB	12	2.52	-21.35	23.74	:	ASN CG	12	2.75	2.75	23.84
ASN OD1	12	2.74	-23.40	24.91	:	ASN ND2	12	3.03	3.03	22.85
ASN C	12	2.17	-21.25	21.29	:	ASN O	12	1.03	1.03	21.53
PRO N	13	2.61	-21.42	20.06	:	PRO CD	13	3.98	3.98	19.67
PRO GA	13	1.81	-21.88	18.93	:	PRO CB	13	2.73	2.73	17.79
PRO CG	13	4.04	-22.16	18.43	:	PRO C	13	1.15	1.15	19.00
PRO O	13	0.33	-23.52	18.17	:	PHE N	14	1.52	1.52	19.91
PHE CA	14	0.98	-25.45	19.99	:	PHE CB	14	2.02	2.02	20.44
PHE CG	14	3.38	-26.29	19.80	:	PHE CD1	14	3.66	3.66	18.58
PHE CD2	14	4.30	-25.52	20.43	:	PHE CE1	14	4.86	4.86	18.03
PHE CE2	14	5.50	-25.25	19.85	:	PHE CZ	14	5.78	5.78	18.66
PHE C	14	-0.16	-25.56	20.96	:	PHE O	14	-0.80	-0.80	21.03
TYR N	15	-0.48	-24.55	21.74	:	TYR CA	15	-1.51	-1.51	22.74
TYR CB	15	-1.04	-23.99	24.00	:	TYR CG	15	-2.10	-2.10	25.04
TYR CD1	15	-2.89	-24.76	25.48	:	TYR CE1	15	-3.83	-3.83	26.45
TYR CD2	15	-2.24	-22.53	25.56	:	TYR CE2	15	-3.17	-3.17	26.52
TYR CZ	15	-3.95	-23.34	26.94	:	TYR OH	15	-4.88	-4.88	27.88
TYR C	15	-2.78	-24.04	22.24	:	TYR O	15	-2.79	-2.79	22.14
PHE N	16	-3.79	-24.86	21.99	:	PHE CA	16	-5.13	-5.13	21.61
PHE CB	16	-5.79	-25.46	20.73	:	PHE CG	16	-5.13	-5.13	19.40
PHE CD1	16	-5.78	-24.67	18.42	:	PHE CD2	16	-3.89	-3.89	19.22
PHE CE1	16	-5.15	-24.53	17.23	:	PHE CE2	16	-3.26	-3.26	18.04
PHE CZ	16	-3.90	-25.08	17.06	:	PHE C	16	-5.97	-5.97	22.86
PHE O	16	-6.47	-25.11	23.52	:	ASN N	17	-6.17	-6.17	23.16
ASN CA	17	-6.76	-22.52	24.39	:	ASN CB	17	-6.43	-6.43	24.56
ASN CG	17	-6.74	-20.63	25.93	:	ASN OD1	17	-6.11	-6.11	26.28
ASN ND2	17	-7.57	-21.19	26.78	:	ASN C	17	-8.22	-8.22	24.31
ASN O	17	-8.80	-22.09	23.39	:	SER N	18	-8.90	-8.90	25.22
SER CA	18	-10.32	-23.45	25.06	:	SER CB	18	-10.82	-10.82	26.02
SER OG	18	-10.32	-23.95	27.25	:	SER C	18	-11.09	-11.09	25.21
SER O	18	-12.27	-22.16	24.86	:	ASP N	19	-10.50	-10.50	25.59
ASP CA	19	-11.38	-19.92	25.67	:	ASP CB	19	-11.09	-11.09	26.89
ASP CG	19	-9.66	-18.65	27.12	:	ASP OD1	19	-8.90	-8.90	26.16
ASP OD2	19	-9.28	-18.47	28.26	:	ASP C	19	-11.36	-11.36	24.38
ASP O	19	-12.23	-18.33	24.14	:	ASN N	20	-10.48	-10.48	23.44
ASN CA	20	-10.77	-18.92	22.13	:	ASN CB	20	-9.90	-9.90	21.92
ASN CG	20	-8.44	-18.06	21.99	:	ASN OD1	20	-8.00	-8.00	21.36
ASN ND2	20	-7.62	-17.36	22.76	:	ASN C	20	-10.63	-10.63	21.00
ASN O	20	-10.65	-19.54	19.85	:	SER N	21	-10.60	-10.60	21.17
SER CA	21	-10.32	-22.16	20.06	:	SER CB	21	-9.12	-9.12	20.37
SER OG	21	-7.95	-22.29	20.01	:	SER C	21	-11.35	-11.35	19.50
SER O	21	-11.02	-23.76	18.51	:	TRP N	22	-12.56	-12.56	20.03
TRP CA	22	-13.55	-24.18	19.55	:	TRP CB	22	-14.17	-14.17	20.68
TRP CG	22	-13.30	-26.06	21.32	:	TRP CD2	22	-13.16	-13.16	20.91
TRP CE2	22	-12.30	-27.84	21.83	:	TRP CE3	22	-13.63	-13.63	19.92
TRP CD1	22	-12.56	-25.81	22.43	:	TRP NE1	22	-11.96	-11.96	22.72
TRP CZ2	22	-11.88	-29.14	21.77	:	TRP CZ3	22	-13.22	-13.22	19.84
TRP CH2	22	-12.36	-29.96	20.77	:	TRP C	22	-14.63	-14.63	18.97
TRP O	22	-14.82	-22.27	19.54	:	ASN N	23	-15.38	-15.38	17.93
ASN CA	23	-16.48	-22.68	17.69	:	ASN CB	23	-16.46	-16.46	16.42
ASN CG	23	-15.17	-21.91	15.61	:	ASN OD1	23	-14.97	-14.97	14.72
ASN ND2	23	-14.30	-20.93	15.85	:	ASN C	23	-17.62	-17.62	17.49
ASN O	23	-17.43	-24.56	16.75	:	THR N	24	-18.70	-18.70	18.22
THR CA	24	-19.99	-23.99	18.24	:	THR CB	24	-20.90	-20.90	19.21

III 12.

THR OG1	24	-20.10	-23.13	20.36	:	THR CG2	24	-22.09	-22.09	19.57
THR C	24	-20.70	-23.98	16.92	:	THR O	24	-20.96	-20.96	16.33
LEU N	25	-21.03	-25.17	16.47	:	LEU CA	25	-21.71	-21.71	15.20
LEU CB	25	-21.18	-26.50	14.51	:	LEU CG	25	-21.94	-21.94	13.40
LEU CD1	25	-21.94	-26.04	12.34	:	LEU CD2	25	-21.35	-21.35	12.92
LEU C	25	-23.17	-25.31	15.56	:	LEU O	25	-23.92	-23.92	14.92
PHE N	26	-23.63	-26.15	16.52	:	PHE CA	26	-25.01	-25.01	16.98
PHE CB	26	-25.77	-27.36	16.40	:	PHE CG	26	-27.18	-27.18	16.95
PHE CD1	26	-28.28	-27.02	16.36	:	PHE CD2	26	-27.36	-27.36	18.05
PHE CE1	26	-29.52	-27.25	16.86	:	PHE CE2	26	-28.60	-28.60	18.54
PHE CZ	26	-29.68	-28.04	17.95	:	PHE C	26	-25.03	-25.03	18.50
PHE O	26	-24.14	-26.94	19.07	:	LYS N	27	-25.99	-25.99	19.20
LYS CA	27	-26.12	-25.93	20.63	:	LYS CB	27	-25.32	-25.32	21.50
LYS CG	27	-25.70	-23.49	21.39	:	LYS CD	27	-25.10	-25.10	22.49
LYS CE	27	-25.27	-21.28	22.17	:	LYS NZ	27	-24.14	-24.14	22.69
LYS C	27	-27.58	-25.63	20.88	:	LYS O	27	-28.17	-28.17	20.29
ASN N	28	-28.17	-26.44	21.72	:	ASN CA	28	-29.55	-29.55	22.09
ASN CB	28	-30.45	-26.99	21.10	:	ASN CG	28	-30.72	-30.72	21.53
ASN ND1	28	-31.67	-28.55	22.24	:	ASN ND2	28	-29.96	-29.96	21.53
ASN C	28	-29.62	-26.85	23.50	:	ASN O	28	-28.60	-28.60	24.01
GLN N	29	-30.79	-26.93	24.11	:	GLN CA	29	-30.78	-30.78	25.49
GLN CB	29	-32.08	-26.99	26.19	:	GLN CG	29	-33.27	-33.27	25.80
GLN CD	29	-33.91	-27.26	24.52	:	GLN OE1	29	-34.74	-34.74	23.94
GLN NE2	29	-33.66	-26.09	23.97	:	GLN C	29	-30.48	-30.48	25.70
GLN O	29	-30.37	-29.15	26.88	:	TYR N	30	-30.35	-30.35	24.65
TYR CA	30	-30.02	-31.00	24.88	:	TYR CB	30	-30.90	-30.90	24.08
TYR CG	30	-32.32	-31.88	24.59	:	TYR CD1	30	-32.70	-32.70	25.66
TYR CE1	30	-34.00	-32.56	26.10	:	TYR CD2	30	-33.19	-33.19	23.93
TYR CE2	30	-34.49	-30.97	24.36	:	TYR CZ	30	-34.90	-34.90	25.44
TYR OH	30	-36.23	-31.63	25.84	:	TYR C	30	-28.61	-28.61	24.58
TYR O	30	-28.22	-32.54	24.90	:	GLY N	31	-27.83	-27.83	23.93
GLY CA	31	-26.44	-30.89	23.69	:	GLY C	31	-25.81	-25.81	22.75
GLY O	31	-26.45	-28.92	22.34	:	HIS N	32	-24.57	-24.57	22.35
HIS CA	32	-23.96	-29.18	21.40	:	HIS CB	32	-23.29	-23.29	22.10
HIS CG	32	-22.26	-28.49	23.13	:	HIS CD2	32	-22.47	-22.47	24.46
HIS ND1	32	-21.07	-29.07	23.01	:	HIS CE1	32	-20.56	-20.56	24.17
HIS NE2	32	-21.42	-28.84	25.02	:	HIS C	32	-22.92	-22.92	20.64
HIS O	32	-22.48	-30.94	21.16	:	ILE N	33	-22.51	-22.51	19.47
ILE CA	33	-21.41	-30.08	18.78	:	ILE CB	33	-21.92	-21.92	17.47
ILE CG2	33	-23.41	-31.12	17.27	:	ILE CG1	33	-21.57	-21.57	16.25
ILE CD1	33	-20.20	-30.72	15.72	:	ILE C	33	-20.51	-20.51	18.49
ILE O	33	-20.99	-27.83	18.00	:	ARG N	34	-19.24	-19.24	18.89
ARG CA	34	-18.32	-27.76	18.55	:	ARG CB	34	-17.69	-17.69	19.81
ARG CG	34	-18.74	-26.44	20.52	:	ARG CD	34	-18.73	-18.73	21.99
ARG NE	34	-17.76	-25.75	22.64	:	ARG CZ	34	-16.93	-16.93	23.57
ARG NH1	34	-16.03	-25.49	24.21	:	ARG NH2	34	-16.93	-16.93	23.85
ARG C	34	-17.21	-28.23	17.60	:	ARG O	34	-16.93	-16.93	17.53
VAL N	35	-16.55	-27.39	16.81	:	VAL CA	35	-15.51	-15.51	15.90
VAL CB	35	-15.93	-27.51	14.48	:	VAL CG1	35	-14.97	-14.97	13.57
VAL CG2	35	-17.30	-28.05	14.14	:	VAL C	35	-14.26	-14.26	16.26
VAL O	35	-14.39	-25.79	16.45	:	LEU N	36	-13.05	-13.05	16.39
LEU CA	36	-11.88	-26.80	16.77	:	LEU CB	36	-10.59	-10.59	16.97
LEU CG	36	-9.77	-27.74	18.26	:	LEU CD1	36	-8.33	-8.33	17.85
LEU CD2	36	-9.94	-26.65	19.25	:	LEU C	36	-11.51	-11.51	15.62
LEU O	36	-11.85	-26.20	14.47	:	GLN N	37	-10.84	-10.84	15.81
GLN CA	37	-10.26	-23.98	14.73	:	GLN CB	37	-9.65	-9.65	15.28
GLN CG	37	-8.57	-22.82	16.32	:	GLN CD	37	-7.59	-7.59	16.16
GLN OE1	37	-7.42	-20.76	16.96	:	GLN NE2	37	-6.95	-6.95	14.99
GLN C	37	-9.19	-24.83	14.03	:	GLN O	37	-8.80	-8.80	14.54

3|32

III. 13

ARG N	38	-8.81	-24.50	12.80	:	ARG CA	38	-7.82	-7.82	12.03
ARG CB	38	-7.59	-24.77	10.65	:	ARG CG	38	-8.76	-8.76	9.82
ARG CD	38	-8.49	-25.08	8.54	:	ARG NE	38	-8.67	-8.67	7.42
ARG CZ	38	-7.62	-23.92	6.68	:	ARG NH1	38	-7.84	-7.84	5.64
ARG NH2	38	-6.40	-24.37	6.96	:	ARG C	38	-6.46	-6.46	12.64
ARG O	38	-6.11	-24.14	13.08	:	PHE N	39	-5.63	-5.63	12.64
PHE CA	39	-4.31	-26.18	13.23	:	PHE CB	39	-3.68	-3.68	13.35
PHE CG	39	-4.49	-28.49	14.22	:	PHE CD1	39	-4.59	-4.59	15.58
PHE CD2	39	-5.10	-29.58	13.67	:	PHE CE1	39	-5.28	-5.28	16.34
PHE CE2	39	-5.80	-30.47	14.44	:	PHE CZ	39	-5.89	-5.89	15.78
PHE C	39	-3.39	-25.31	12.41	:	PHE O	39	-2.72	-2.72	13.01
ASP N	40	-3.28	-25.35	11.09	:	ASP CA	40	-2.37	-2.37	10.35
ASP CB	40	-2.12	-25.10	8.97	:	ASP CG	40	-3.36	-3.36	8.12
ASP OD1	40	-4.42	-25.50	8.54	:	ASP OD2	40	-3.32	-3.32	7.05
ASP C	40	-2.92	-23.07	10.27	:	ASP O	40	-2.17	-2.17	10.03
GLN N	41	-4.18	-22.75	10.44	:	GLN CA	41	-4.61	-4.61	10.65
GLN CB	41	-6.09	-21.15	10.99	:	GLN CG	41	-6.70	-6.70	10.03
GLN CD	41	-6.79	-20.69	8.57	:	GLN OE1	41	-5.81	-5.81	7.87
GLN NE2	41	-8.01	-20.84	8.01	:	GLN C	41	-3.95	-3.95	11.88
GLN O	41	-3.75	-19.62	11.98	:	GLN N	42	-3.69	-3.69	12.89
GLN CA	42	-3.12	-21.09	14.10	:	GLN CB	42	-3.40	-3.40	15.16
GLN CG	42	-3.74	-21.17	16.29	:	GLN CD	42	-3.06	-3.06	17.58
GLN OE1	42	-3.57	-21.23	18.66	:	GLN NE2	42	-1.90	-1.90	17.48
GLN C	42	-1.65	-20.83	14.03	:	GLN O	42	-1.15	-1.15	14.70
SER N	43	-0.91	-21.60	13.28	:	SER CA	43	0.53	0.53	13.15
SER CB	43	1.20	-22.10	14.34	:	SER OG	43	2.53	2.53	14.44
SER C	43	0.93	-22.23	11.90	:	SER O	43	0.60	0.60	11.85
LYS N	44	1.63	-21.73	10.89	:	LYS CA	44	2.00	2.00	9.81
LYS CB	44	2.54	-21.89	8.55	:	LYS CG	44	1.57	1.57	7.30
LYS CD	44	0.61	-23.38	7.21	:	LYS CE	44	0.14	0.14	5.83
LYS NZ	44	-0.82	-25.21	5.93	:	LYS C	44	3.06	3.06	10.32
LYS O	44	3.42	-24.51	9.60	:	ARG N	45	3.55	3.55	11.58
ARG CA	45	4.42	-24.48	12.14	:	ARG CB	45	4.86	4.86	13.55
ARG CG	45	5.34	-22.96	13.90	:	ARG CD	45	5.97	5.97	15.24
ARG NE	45	6.53	-21.95	15.79	:	ARG CZ	45	7.50	7.50	16.70
ARG NH1	45	7.91	-20.90	17.29	:	ARG NH2	45	8.14	8.14	16.95
ARG C	45	3.58	-25.73	12.24	:	ARG O	45	4.11	4.11	12.07
LEU N	46	2.27	-25.71	12.50	:	LEU CA	46	1.49	1.49	12.63
LEU CB	46	0.35	-26.72	13.61	:	LEU CG	46	0.82	0.82	14.97
LEU CD1	46	-0.32	-25.71	15.73	:	LEU CD2	46	1.45	1.45	15.57
LEU C	46	0.92	-27.25	11.29	:	LEU O	46	-0.18	-0.18	11.21
GLN N	47	1.68	-27.00	10.23	:	GLN CA	47	1.24	1.24	8.85
GLN CB	47	2.29	-26.70	7.94	:	GLN CG	47	2.40	2.40	6.62
GLN CD	47	3.30	-26.44	5.80	:	GLN OE1	47	3.17	3.17	5.89
GLN NE2	47	4.19	-27.04	4.99	:	GLN C	47	0.90	0.90	8.48
GLN O	47	-0.08	-28.81	7.80	:	ASN N	48	1.70	1.70	8.82
ASN CA	48	1.32	-30.94	8.49	:	ASN CB	48	2.51	2.51	8.77
ASN CG	48	3.46	-31.75	7.59	:	ASN OD1	48	4.39	4.39	7.54
ASN ND2	48	3.35	-30.92	6.56	:	ASN C	48	0.09	0.09	9.19
ASN O	48	-0.28	-32.65	9.00	:	LEU N	49	-0.62	-0.62	9.96
LEU CA	49	-1.82	-31.14	10.59	:	LEU CB	49	-1.76	-1.76	12.01
LEU CG	49	-1.80	-31.74	13.09	:	LEU CD1	49	-1.09	-1.09	12.69
LEU CD2	49	-1.14	-31.18	14.30	:	LEU C	49	-2.87	-2.87	9.81
LEU O	49	-3.92	-30.23	10.38	:	GLU N	50	-2.80	-2.80	8.53
GLU CA	50	-3.82	-29.18	7.92	:	GLU CB	50	-3.15	-3.15	6.80
GLU CG	50	-3.92	-27.75	5.68	:	GLU CD	50	-3.02	-3.02	4.48
GLU OE1	50	-3.35	-26.28	3.88	:	GLU OE2	50	-1.97	-1.97	4.19
GLU C	50	-5.01	-29.96	7.47	:	GLU O	50	-6.14	-6.14	7.44
ASP N	51	-4.78	-31.25	7.31	:	ASP CA	51	-5.81	-5.81	6.88

4/32

III 1.4

ASP CB	51	-5.21	-33.38	6.26	:	ASP CG	51	-4.26	-4.26	5.11
ASP OD1	51	-4.68	-32.36	4.21	:	ASP OD2	51	-3.13	-3.13	5.12
ASP C	51	-6.64	-32.67	8.05	:	ASP O	51	-7.47	-7.47	7.84
TYR N	52	-6.48	-32.28	9.31	:	TYR CA	52	-7.23	-7.23	10.37
TYR CB	52	-6.35	-33.60	11.31	:	TYR CG	52	-5.58	-5.58	10.63
TYR CD1	52	-6.01	-35.97	10.64	:	TYR CE1	52	-5.26	-5.26	10.04
TYR CD2	52	-4.41	-34.37	10.01	:	TYR CE2	52	-3.65	-3.65	9.41
TYR CZ	52	-4.08	-36.63	9.44	:	TYR OH	52	-3.31	-3.31	8.87
TYR C	52	-8.01	-31.94	11.14	:	TYR O	52	-7.57	-7.57	11.23
ARG N	53	-9.18	-32.31	11.63	:	ARG CA	53	-9.95	-9.95	12.48
ARG CB	53	-11.20	-30.94	11.82	:	ARG CG	53	-10.97	-10.97	10.52
ARG CD	53	-10.20	-28.99	10.71	:	ARG NE	53	-11.08	-11.08	10.16
ARG CZ	53	-11.71	-27.11	10.92	:	ARG NH1	53	-12.62	-12.62	10.40
ARG NH2	53	-11.34	-26.97	12.18	:	ARG C	53	-10.39	-10.39	13.68
ARG O	53	-10.49	-33.40	13.59	:	LEU N	54	-10.69	-10.69	14.82
LEU CA	54	-11.18	-32.37	15.95	:	LEU CB	54	-10.49	-10.49	17.21
LEU CG	54	-9.16	-32.50	17.67	:	LEU CD1	54	-8.80	-8.80	18.94
LEU CD2	54	-9.23	-33.94	18.03	:	LEU C	54	-12.60	-12.60	16.05
LEU O	54	-12.77	-30.67	15.94	:	VAL N	55	-13.67	-13.67	16.15
VAL CA	55	-14.98	-32.07	16.45	:	VAL CB	55	-15.94	-15.94	15.18
VAL CG1	55	-15.35	-32.84	14.04	:	VAL CG2	55	-17.26	-17.26	15.53
VAL C	55	-15.54	-32.84	17.66	:	VAL O	55	-15.45	-15.45	17.68
GLU N	56	-16.10	-32.14	18.67	:	GLU CA	56	-16.47	-16.47	19.99
GLU CB	56	-15.64	-31.75	20.92	:	GLU CG	56	-16.00	-16.00	22.37
GLU CD	56	-17.12	-30.40	22.55	:	GLU OE1	56	-17.85	-17.85	23.55
GLU OE2	56	-17.28	-29.52	21.73	:	GLU C	56	-17.97	-17.97	20.17
GLU O	56	-18.56	-31.67	19.53	:	PHE N	57	-18.66	-18.66	20.98
PHE CA	57	-20.12	-33.36	21.06	:	PHE CB	57	-20.69	-20.69	20.13
PHE CG	57	-22.15	-34.85	20.30	:	PHE CD1	57	-22.47	-22.47	20.95
PHE CD2	57	-23.20	-34.13	19.74	:	PHE CE1	57	-23.79	-23.79	21.01
PHE CE2	57	-24.52	-34.54	19.80	:	PHE CZ	57	-24.82	-24.82	20.44
PHE C	57	-20.49	-33.75	22.45	:	PHE O	57	-19.78	-19.78	22.97
ARG N	58	-21.54	-33.24	23.07	:	ARG CA	58	-22.03	-22.03	24.32
ARG CB	58	-21.52	-33.05	25.54	:	ARG CG	58	-22.43	-22.43	26.44
ARG CD	58	-22.44	-32.83	27.83	:	ARG NE	58	-21.29	-21.29	28.65
ARG CZ	58	-21.23	-32.75	29.99	:	ARG NH1	58	-20.14	-20.14	30.71
ARG NH2	58	-22.26	-33.31	30.65	:	ARG C	58	-23.51	-23.51	24.26
ARG O	58	-23.97	-32.66	23.69	:	SER N	59	-24.26	-24.26	24.84
SER CA	59	-25.70	-34.48	24.82	:	SER CB	59	-26.24	-26.24	23.60
SER OG	59	-25.92	-36.63	23.38	:	SER C	59	-26.21	-26.21	26.12
SER O	59	-25.56	-35.97	26.72	:	LYS N	60	-27.36	-27.36	26.58
LYS CA	60	-27.95	-35.01	27.84	:	LYS CB	60	-29.05	-29.05	28.11
LYS CG	60	-28.58	-32.53	27.99	:	LYS CD	60	-28.62	-28.62	29.24
LYS CE	60	-28.33	-32.42	30.58	:	LYS NZ	60	-27.17	-27.17	30.57
LYS C	60	-28.47	-36.48	27.77	:	LYS O	60	-28.50	-28.50	26.67
PRO N	61	-28.82	-37.21	28.84	:	PRO CD	61	-28.43	-28.43	30.20
PRO CA	61	-29.53	-38.49	28.85	:	PRO CB	61	-30.02	-30.02	30.22
PRO CG	61	-28.81	-38.18	30.92	:	PRO C	61	-30.66	-30.66	27.87
PRO O	61	-31.36	-37.70	27.57	:	GLU N	62	-30.84	-30.84	27.42
GLU CA	62	-31.89	-40.28	26.47	:	GLU CB	62	-33.19	-33.19	27.26
GLU CG	62	-32.93	-41.46	28.44	:	GLU CD	62	-34.16	-34.16	29.02
GLU OE1	62	-34.25	-43.38	29.02	:	GLU OE2	62	-35.03	-35.03	29.49
GLU C	62	-32.07	-39.25	25.37	:	GLU O	62	-33.08	-33.08	25.26
THR N	63	-31.07	-39.08	24.51	:	THR CA	63	-31.17	-31.17	23.50
THR CB	63	-30.28	-36.96	24.10	:	THR OG1	63	-30.78	-30.78	23.73
THR CG2	63	-28.84	-37.20	23.71	:	THR C	63	-30.77	-30.77	22.14
THR O	63	-30.02	-39.56	22.14	:	LEU N	64	-31.22	-31.22	20.97
LEU CA	64	-30.75	-38.64	19.68	:	LEU CB	64	-31.87	-31.87	18.98
LEU CG	64	-31.85	-39.57	17.47	:	LEU CD1	64	-31.67	-31.67	17.07

5/32

III . 1.5 .

LEU CD2	64	-33.14	-39.04	16.91	:	LEU C	64	-30.34	-30.34	18.82
LEU O	64	-30.94	-36.37	18.89	:	LEU N	65	-29.24	-29.24	18.08
LEU CA	65	-28.80	-36.62	17.12	:	LEU CB	65	-27.28	-27.28	17.14
LEU CG	65	-26.49	-35.91	16.09	:	LEU CD1	65	-26.66	-26.66	16.27
LEU CD2	65	-25.06	-36.34	16.20	:	LEU C	65	-29.43	-29.43	15.79
LEU O	65	-29.30	-38.24	15.47	:	LEU N	66	-30.21	-30.21	15.06
LEU CA	66	-30.87	-36.62	13.82	:	LEU CB	66	-31.81	-31.81	13.47
LEU CG	66	-32.99	-35.29	14.43	:	LEU CD1	66	-33.71	-33.71	14.12
LEU CD2	66	-33.97	-36.44	14.28	:	LEU C	66	-29.95	-29.95	12.65
LEU O	66	-28.78	-36.57	12.70	:	PRO N	67	-30.38	-30.38	11.60
PRO CD	67	-31.65	-38.37	11.53	:	PRO CA	67	-29.51	-29.51	10.53
PRO CB	67	-30.42	-38.92	9.64	:	PRO CG	67	-31.33	-31.33	10.62
PRO C	67	-28.69	-37.16	9.73	:	PRO O	67	-29.27	-29.27	9.20
GLN N	68	-27.38	-37.32	9.57	:	GLN CA	68	-26.54	-26.54	8.70
GLN CB	68	-25.81	-35.55	9.57	:	GLN CG	68	-24.60	-24.60	10.22
GLN CD	68	-24.11	-35.37	11.37	:	GLN OE1	68	-24.18	-24.18	12.49
GLN NE2	68	-23.63	-34.17	11.13	:	GLN C	68	-25.51	-25.51	7.82
GLN O	68	-25.41	-38.41	7.97	:	GLN N	69	-24.76	-24.76	6.92
GLN CA	69	-23.57	-37.19	6.28	:	GLN CB	69	-23.47	-23.47	4.80
GLN CG	69	-24.66	-37.75	4.14	:	GLN CD	69	-25.24	-25.24	3.37
GLN OE1	69	-24.53	-35.78	2.80	:	GLN NE2	69	-26.56	-26.56	3.31
GLN C	69	-22.47	-36.15	6.42	:	GLN O	69	-22.77	-22.77	6.30
ALA N	70	-21.20	-36.45	6.63	:	ALA CA	70	-20.21	-20.21	6.66
ALA CB	70	-19.41	-35.44	7.93	:	ALA C	70	-19.24	-19.24	5.53
ALA O	70	-18.97	-36.70	5.18	:	ASP N	71	-18.64	-18.64	4.91
ASP CA	71	-17.63	-34.86	3.92	:	ASP CB	71	-17.43	-17.43	2.94
ASP CG	71	-17.03	-32.37	3.54	:	ASP OD1	71	-16.21	-16.21	2.95
ASP OD2	71	-17.56	-32.02	4.58	:	ASP C	71	-16.33	-16.33	4.61
ASP O	71	-15.28	-34.87	4.06	:	ALA N	72	-16.23	-16.23	5.70
ALA CA	72	-14.96	-36.17	6.35	:	ALA CB	72	-14.79	-14.79	7.50
ALA C	72	-14.88	-37.54	6.91	:	ALA O	72	-15.90	-15.90	7.39
GLU N	73	-13.79	-38.27	6.96	:	GLU CA	73	-13.71	-13.71	7.63
GLU CB	73	-12.44	-40.11	7.17	:	GLU CG	73	-11.95	-11.95	7.68
GLU CD	73	-12.40	-42.58	6.80	:	GLU OE1	73	-11.99	-11.99	7.22
GLU OE2	73	-13.12	-42.37	5.77	:	GLU C	73	-13.71	-13.71	9.14
GLU O	73	-13.00	-38.37	9.53	:	LEU N	74	-14.42	-14.42	10.05
LEU CA	74	-14.55	-39.60	11.46	:	LEU CB	74	-15.98	-15.98	11.78
LEU CG	74	-16.55	-37.93	11.81	:	LEU CD1	74	-15.97	-15.97	10.75
LEU CD2	74	-18.02	-38.04	11.60	:	LEU C	74	-14.09	-14.09	12.32
LEU O	74	-14.51	-41.85	12.05	:	LEU N	75	-13.21	-13.21	13.29
LEU CA	75	-12.84	-41.55	14.24	:	LEU CB	75	-11.35	-11.35	14.31
LEU CG	75	-10.68	-42.43	15.40	:	LEU CD1	75	-11.37	-11.37	15.82
LEU CD2	75	-9.43	-42.91	14.82	:	LEU C	75	-13.49	-13.49	15.46
LEU O	75	-13.13	-39.88	15.96	:	LEU N	76	-14.58	-14.58	15.82
LEU CA	76	-15.55	-41.26	16.86	:	LEU CB	76	-16.84	-16.84	16.40
LEU CG	76	-18.23	-41.53	16.75	:	LEU CD1	76	-18.44	-18.44	18.21
LEU CD2	76	-18.48	-40.13	16.31	:	LEU C	76	-14.95	-14.95	18.10
LEU O	76	-14.58	-43.03	17.97	:	VAL N	77	-14.79	-14.79	19.26
VAL CA	77	-14.18	-41.82	20.47	:	VAL CB	77	-12.78	-12.78	20.72
VAL CG1	77	-12.27	-41.63	22.08	:	VAL CG2	77	-11.83	-11.83	19.84
VAL C	77	-15.01	-41.44	21.67	:	VAL O	77	-15.33	-15.33	21.80
VAL N	78	-15.37	-42.31	22.60	:	VAL CA	78	-16.21	-16.21	23.68
VAL CB	78	-17.25	-42.95	23.93	:	VAL CG1	78	-18.19	-18.19	25.01
VAL CG2	78	-18.12	-43.15	22.73	:	VAL C	78	-15.44	-15.44	24.94
VAL O	78	-14.84	-42.35	25.55	:	ARG N	79	-15.30	-15.30	25.36
ARG CA	79	-14.86	-39.95	26.71	:	ARG CB	79	-14.43	-14.43	26.82
ARG CG	79	-14.02	-37.74	25.58	:	ARG CD	79	-14.70	-14.70	25.37
ARG NE	79	-13.74	-35.32	25.50	:	ARG CZ	79	-13.99	-13.99	25.33
ARG NH1	79	-13.07	-33.09	25.61	:	ARG NH2	79	-15.17	-15.17	24.82

6/32

III - 16.

ARG C	79	-16.20	-40.10	27.50	:	ARG O	79	-17.24	-17.24	26.90
SER N	80	-16.49	-40.50	28.75	:	SER CA	80	-17.91	-17.91	29.29
SER CB	80	-18.40	-39.17	29.61	:	SER OG	80	-17.56	-17.56	30.62
SER C	80	-19.07	-41.27	28.53	:	SER O	80	-19.95	-19.95	27.93
GLY N	81	-18.96	-42.60	28.70	:	GLY CA	81	-19.64	-19.64	28.06
GLY C	81	-21.11	-43.61	27.77	:	GLY O	81	-21.73	-21.73	28.31
SER N	82	-21.62	-44.58	26.99	:	SER CA	82	-23.00	-23.00	26.46
SER CB	82	-23.92	-43.63	26.88	:	SER OG	82	-23.45	-23.45	26.23
SER C	82	-23.01	-44.67	24.89	:	SER O	82	-22.00	-22.00	24.31
ALA N	83	-23.96	-44.07	24.15	:	ALA CA	83	-23.96	-23.96	22.68
ALA CB	83	-22.71	-43.47	22.06	:	ALA C	83	-24.11	-24.11	21.88
ALA O	83	-23.33	-46.28	21.95	:	ILE N	84	-25.16	-25.16	21.09
ILE CA	84	-25.51	-46.45	20.19	:	ILE CB	84	-26.99	-26.99	20.33
ILE CG2	84	-27.43	-47.70	19.14	:	ILE CG1	84	-27.19	-27.19	21.63
ILE CD1	84	-28.67	-47.63	22.03	:	ILE C	84	-25.32	-25.32	18.87
ILE O	84	-25.98	-44.71	18.65	:	LEU N	85	-24.51	-24.51	17.94
LEU CA	85	-24.36	-45.46	16.70	:	LEU CB	85	-22.90	-22.90	16.51
LEU CG	85	-22.27	-44.83	15.24	:	LEU CD1	85	-22.67	-22.67	14.86
LEU CD2	85	-20.78	-45.01	15.45	:	LEU C	85	-24.93	-24.93	15.64
LEU O	85	-24.79	-47.57	15.74	:	VAL N	86	-25.60	-25.60	14.65
VAL CA	86	-26.00	-46.71	13.56	:	VAL CB	86	-27.56	-27.56	13.57
VAL CG1	86	-28.28	-46.04	14.42	:	VAL CG2	86	-28.15	-28.15	12.19
VAL C	86	-25.55	-46.05	12.27	:	VAL O	86	-25.74	-25.74	12.14
LEU N	87	-24.88	-46.77	11.38	:	LEU CA	87	-24.55	-24.55	10.11
LEU CB	87	-23.25	-46.65	9.61	:	LEU CG	87	-22.11	-22.11	10.54
LEU CD1	87	-20.93	-47.07	9.70	:	LEU CD2	87	-21.85	-21.85	11.28
LEU C	87	-25.66	-46.73	9.22	:	LEU O	87	-26.00	-26.00	9.39
VAL N	88	-26.30	-45.98	8.31	:	VAL CA	88	-27.35	-27.35	7.46
VAL CB	88	-28.47	-45.49	7.41	:	VAL CG1	88	-29.45	-29.45	6.38
VAL CG2	88	-29.12	-45.33	8.76	:	VAL C	88	-26.69	-26.69	6.11
VAL O	88	-26.15	-45.62	5.66	:	LYS N	89	-26.65	-26.65	5.38
LYS CA	89	-25.94	-47.80	4.10	:	LYS CB	89	-25.02	-25.02	4.15
LYS CG	89	-23.71	-48.54	4.77	:	LYS CD	89	-22.73	-22.73	5.27
LYS CE	89	-21.54	-48.85	5.96	:	LYS NZ	89	-20.87	-20.87	7.05
LYS C	89	-26.98	-47.86	2.97	:	LYS O	89	-28.07	-28.07	3.24
PRO N	90	-26.80	-47.35	1.74	:	PRO CD	90	-25.54	-25.54	1.17
PRO CA	90	-27.81	-47.17	0.73	:	PRO CB	90	-27.18	-27.18	-0.39
PRO CG	90	-25.82	-46.96	-0.33	:	PRO C	90	-28.36	-28.36	0.26
PRO O	90	-29.58	-48.64	0.08	:	ASP N	91	-27.55	-27.55	0.14
ASP CA	91	-28.01	-50.83	-0.22	:	ASP CB	91	-26.81	-26.81	-0.70
ASP CG	91	-25.71	-51.69	0.33	:	ASP OD1	91	-25.45	-25.45	1.04
ASP OD2	91	-25.10	-52.76	0.44	:	ASP C	91	-28.68	-28.68	0.95
ASP O	91	-28.25	-52.60	1.40	:	ASP N	92	-29.73	-29.73	1.52
ASP CA	92	-30.47	-51.44	2.66	:	ASP CB	92	-31.47	-31.47	2.22
ASP CG	92	-32.80	-52.49	2.95	:	ASP OD1	92	-33.66	-33.66	2.43
ASP OD2	92	-33.06	-51.80	3.97	:	ASP C	92	-29.68	-29.68	3.77
ASP O	92	-30.30	-52.74	4.60	:	ARG N	93	-28.36	-28.36	3.91
ARG CA	93	-27.71	-52.49	5.11	:	ARG CB	93	-26.24	-26.24	4.79
ARG CG	93	-25.90	-53.91	3.68	:	ARG CD	93	-24.33	-24.33	3.58
ARG NE	93	-23.80	-54.65	4.89	:	ARG CZ	93	-23.11	-23.11	5.89
ARG NH1	93	-22.86	-54.55	7.10	:	ARG NH2	93	-22.59	-22.59	5.67
ARG C	93	-27.82	-51.43	6.22	:	ARG O	93	-28.34	-28.34	6.03
ARG N	94	-27.38	-51.77	7.43	:	ARG CA	94	-27.28	-27.28	8.64
ARG CB	94	-28.49	-51.02	9.53	:	ARG CG	94	-29.32	-29.32	9.54
ARG CD	94	-30.26	-49.70	8.35	:	ARG NE	94	-31.09	-31.09	8.24
ARG CZ	94	-31.62	-51.29	7.06	:	ARG NH1	94	-32.34	-32.34	6.95
ARG NH2	94	-31.49	-50.56	5.96	:	ARG C	94	-26.14	-26.14	9.46
ARG O	94	-25.65	-52.66	9.15	:	GLU N	95	-25.69	-25.69	10.48
GLU CA	95	-24.63	-51.38	11.31	:	GLU CB	95	-23.30	-23.30	10.84

7/32

III - 1.7

GLU CG	95	-22.38	-52.01	10.37	:	GLU CD	95	-21.96	-21.96	8.93
GLU OE1	95	-20.79	-51.95	8.57	:	GLU OE2	95	-22.78	-22.78	8.07
GLU C	95	-24.95	-50.70	12.61	:	GLU O	95	-25.21	-25.21	12.58
TYR N	96	-24.98	-51.44	13.73	:	TYR CA	96	-25.32	-25.32	15.06
TYR CB	96	-26.41	-51.68	15.76	:	TYR CG	96	-27.66	-27.66	14.92
TYR CD1	96	-28.61	-50.70	15.19	:	TYR CE1	96	-29.68	-29.68	14.35
TYR CD2	96	-27.76	-52.44	13.82	:	TYR CE2	96	-28.81	-28.81	12.98
TYR CZ	96	-29.76	-51.34	13.24	:	TYR OH	96	-30.78	-30.78	12.33
TYR C	96	-24.06	-51.07	15.88	:	TYR O	96	-23.50	-23.50	15.91
PHE N	97	-23.49	-50.03	16.46	:	PHE CA	97	-22.41	-22.41	17.38
PHE CB	97	-21.24	-49.51	17.00	:	PHE CG	97	-20.75	-20.75	15.64
PHE CD1	97	-21.31	-49.23	14.59	:	PHE CD2	97	-19.75	-19.75	15.50
PHE CE1	97	-20.82	-49.51	13.36	:	PHE CE2	97	-19.27	-19.27	14.27
PHE CZ	97	-19.81	-50.43	13.20	:	PHE C	97	-22.88	-22.88	18.70
PHE O	97	-23.58	-48.66	18.77	:	PHE N	98	-22.55	-22.55	19.80
PHE CA	98	-22.81	-49.88	21.13	:	PHE CB	98	-23.49	-23.49	21.97
PHE CG	98	-23.71	-50.44	23.39	:	PHE CD1	98	-24.78	-24.78	23.67
PHE CD2	98	-22.85	-50.81	24.41	:	PHE CE1	98	-24.98	-24.98	24.96
PHE CE2	98	-23.04	-50.38	25.70	:	PHE CZ	98	-24.12	-24.12	25.97
PHE C	98	-21.37	-49.65	21.57	:	PHE O	98	-20.53	-20.53	21.59
LEU N	99	-21.13	-48.36	21.70	:	LEU CA	99	-19.85	-19.85	22.04
LEU CB	99	-19.68	-46.53	21.20	:	LEU CG	99	-18.81	-18.81	19.97
LEU CD1	99	-19.04	-47.67	19.14	:	LEU CD2	99	-19.12	-19.12	19.19
LEU C	99	-19.93	-47.49	23.54	:	LEU O	99	-21.02	-21.02	24.08
THR N	100	-18.86	-47.28	24.29	:	THR CA	100	-18.87	-18.87	25.67
THR CB	100	-19.58	-47.78	26.62	:	THR OG1	100	-19.74	-19.74	27.76
THR CG2	100	-18.88	-49.07	27.01	:	THR C	100	-17.42	-17.42	26.16
THR O	100	-16.60	-47.53	25.72	:	SER N	101	-17.13	-17.13	27.10
SER CA	101	-15.75	-45.57	27.49	:	SER CB	101	-15.63	-15.63	28.52
SER OG	101	-16.16	-44.81	29.79	:	SER C	101	-15.00	-15.00	28.07
SER O	101	-15.63	-47.76	28.43	:	ASP N	102	-13.66	-13.66	28.11
ASP CA	102	-12.69	-47.42	28.83	:	ASP CB	102	-12.75	-12.75	30.25
ASP CG	102	-13.60	-47.61	31.27	:	ASP OD1	102	-14.77	-14.77	30.97
ASP OD2	102	-13.01	-47.94	32.32	:	ASP C	102	-12.83	-12.83	28.77
ASP O	102	-12.99	-49.56	27.67	:	ASN N	103	-12.59	-12.59	29.88
ASN CA	103	-12.92	-51.11	30.03	:	ASN CB	103	-12.58	-12.58	31.45
ASN CG	103	-13.56	-50.80	32.49	:	ASN OD1	103	-13.21	-13.21	33.68
ASN ND2	103	-14.73	-50.15	32.37	:	ASN C	103	-14.40	-14.40	29.72
ASN O	103	-15.33	-50.69	29.83	:	PRO N	104	-14.72	-14.72	29.51
PRO CD	104	-15.18	-53.63	30.64	:	PRO CA	104	-14.17	-14.17	28.44
PRO CB	104	-13.35	-54.64	29.25	:	PRO CG	104	-14.34	-14.34	30.42
PRO C	104	-15.33	-54.33	27.65	:	PRO O	104	-16.50	-16.50	27.93
ILE N	105	-15.07	-55.33	26.75	:	ILE CA	105	-16.08	-16.08	25.86
ILE CB	105	-16.66	-57.27	26.63	:	ILE CG2	105	-17.34	-17.34	27.98
ILE CG1	105	-17.66	-58.03	25.68	:	ILE CD1	105	-17.03	-17.03	24.74
ILE C	105	-17.21	-55.05	25.35	:	ILE O	105	-18.41	-18.41	25.61
PHE N	106	-16.74	-53.92	24.75	:	PHE CA	106	-17.58	-17.58	24.07
PHE CB	106	-18.48	-52.14	25.06	:	PHE CG	106	-19.83	-19.83	25.17
PHE CD1	106	-20.28	-53.69	24.14	:	PHE CD2	106	-20.57	-20.57	26.33
PHE CE1	106	-21.47	-54.41	24.27	:	PHE CE2	106	-21.75	-21.75	26.45
PHE CZ	106	-22.21	-54.28	25.44	:	PHE C	106	-16.93	-16.93	23.13
PHE O	106	-17.52	-51.66	22.05	:	SER N	107	-15.73	-15.73	23.38
SER CA	107	-15.09	-50.38	22.50	:	SER CB	107	-15.18	-15.18	20.98
SER OG	107	-14.04	-50.06	20.37	:	SER C	107	-15.70	-15.70	22.67
SER O	107	-16.90	-48.77	22.83	:	ASP N	108	-14.70	-14.70	22.76
ASP CA	108	-14.95	-46.76	22.94	:	ASP CB	108	-14.05	-14.05	24.02
ASP CG	108	-12.55	-46.26	23.80	:	ASP OD1	108	-11.87	-11.87	24.62
ASP OD2	108	-12.00	-46.87	22.86	:	ASP C	108	-14.74	-14.74	21.65
ASP O	108	-14.81	-44.84	21.62	:	HIS N	109	-14.51	-14.51	20.54

8/32

III. 18.

HIS CA	109	-14.47	-45.96	19.31	:	HIS CB	109	-13.14	-13.14	18.95
HIS CG	109	-12.21	-46.61	19.00	:	HIS CD2	109	-11.61	-11.61	17.95
HIS ND1	109	-11.80	-47.13	20.13	:	HIS CE1	109	-10.92	-10.92	19.84
HIS NE2	109	-10.81	-48.11	18.52	:	HIS C	109	-14.94	-14.94	18.07
HIS O	109	-15.10	-47.83	18.08	:	GLN N	110	-15.06	-15.06	16.97
GLN CA	110	-15.62	-46.48	15.78	:	GLN CB	110	-17.11	-17.11	16.04
GLN CG	110	-17.80	-47.48	14.97	:	GLN CD	110	-17.02	-17.02	14.40
GLN OE1	110	-16.83	-48.73	13.20	:	GLN NE2	110	-16.49	-16.49	15.14
GLN C	110	-15.33	-45.49	14.67	:	GLN O	110	-15.29	-15.29	14.92
LYS N	111	-15.06	-45.99	13.48	:	LYS CA	111	-14.74	-14.74	12.34
LYS CB	111	-13.62	-45.88	11.64	:	LYS CG	111	-13.16	-13.16	10.33
LYS CD	111	-12.32	-46.31	9.49	:	LYS CE	111	-11.20	-11.20	10.35
LYS NZ	111	-9.93	-47.28	9.70	:	LYS C	111	-15.99	-15.99	11.48
LYS O	111	-16.47	-46.07	10.95	:	ILE N	112	-16.58	-16.58	11.34
ILE CA	112	-17.76	-43.75	10.51	:	ILE CB	112	-18.60	-18.60	11.06
ILE CG2	112	-19.90	-42.58	10.27	:	ILE CG1	112	-18.83	-18.83	12.53
ILE CD1	112	-19.66	-41.59	13.03	:	ILE C	112	-17.18	-17.18	9.13
ILE O	112	-16.49	-42.41	9.10	:	PRO N	113	-17.31	-17.31	7.98
PRO CD	113	-18.03	-45.26	7.79	:	PRO CA	113	-16.49	-16.49	6.82
PRO CB	113	-16.58	-44.96	6.01	:	PRO CG	113	-17.03	-17.03	6.98
PRO C	113	-16.94	-42.47	6.08	:	PRO O	113	-18.13	-18.13	6.09
ALA N	114	-16.15	-41.73	5.35	:	ALA CA	114	-16.62	-16.62	4.74
ALA CB	114	-15.47	-39.96	3.92	:	ALA C	114	-17.91	-17.91	3.92
ALA O	114	-17.91	-40.47	2.70	:	GLY N	115	-19.07	-19.07	4.50
GLY CA	115	-20.23	-39.80	3.73	:	GLY C	115	-21.33	-21.33	4.04
GLY O	115	-22.33	-40.62	3.36	:	THR N	116	-21.16	-21.16	5.00
THR CA	116	-22.15	-42.66	5.54	:	THR CB	116	-21.62	-21.62	6.54
THR OG1	116	-20.35	-44.09	6.13	:	THR CG2	116	-22.37	-22.37	6.51
THR C	116	-23.11	-41.88	6.39	:	THR O	116	-22.63	-22.63	7.11
ILE N	117	-24.40	-42.15	6.31	:	ILE CA	117	-25.35	-25.35	7.14
ILE CB	117	-26.70	-41.56	6.42	:	ILE CG2	117	-27.84	-27.84	7.40
ILE CG1	117	-26.83	-40.39	5.47	:	ILE CD1	117	-28.22	-28.22	4.94
ILE C	117	-25.33	-42.10	8.52	:	ILE O	117	-25.25	-25.25	8.59
PHE N	118	-25.40	-41.42	9.65	:	PHE CA	118	-25.34	-25.34	10.93
PHE CB	118	-23.88	-42.14	11.46	:	PHE CG	118	-23.14	-23.14	11.78
PHE CD1	118	-23.21	-40.33	13.06	:	PHE CD2	118	-22.47	-22.47	10.81
PHE CE1	118	-22.61	-39.14	13.35	:	PHE CE2	118	-21.87	-21.87	11.12
PHE CZ	118	-21.94	-38.47	12.38	:	PHE C	118	-26.24	-26.24	11.90
PHE O	118	-26.40	-40.18	11.74	:	TYR N	119	-26.89	-26.89	12.87
TYR CA	119	-27.52	-41.17	13.89	:	TYR CB	119	-29.07	-29.07	13.80
TYR CG	119	-29.81	-42.53	13.49	:	TYR CD1	119	-29.75	-29.75	12.23
TYR CE1	119	-30.40	-44.23	12.00	:	TYR CD2	119	-30.50	-30.50	14.50
TYR CE2	119	-31.15	-44.38	14.27	:	TYR CZ	119	-31.08	-31.08	13.00
TYR OH	119	-31.57	-46.13	12.70	:	TYR C	119	-27.01	-27.01	15.20
TYR O	119	-26.45	-42.78	15.23	:	LEU N	120	-27.11	-27.11	16.31
LEU CA	120	-26.42	-41.44	17.53	:	LEU CB	120	-25.31	-25.31	17.83
LEU CG	120	-23.86	-40.75	17.90	:	LEU CD1	120	-23.09	-23.09	17.72
LEU CD2	120	-23.50	-41.32	19.23	:	LEU C	120	-27.47	-27.47	18.62
LEU O	120	-28.22	-40.39	18.55	:	VAL N	121	-27.70	-27.70	19.56
VAL CA	121	-28.66	-41.97	20.61	:	VAL CB	121	-29.94	-29.94	20.60
VAL CG1	121	-30.11	-43.46	19.21	:	VAL CG2	121	-29.89	-29.89	21.59
VAL C	121	-27.88	-42.08	21.90	:	VAL O	121	-26.85	-26.85	21.88
ASN N	122	-28.22	-41.40	23.00	:	ASN CA	122	-27.49	-27.49	24.27
ASN CB	122	-27.36	-40.18	25.06	:	ASN CG	122	-26.75	-26.75	26.48
ASN OD1	122	-26.35	-41.42	26.91	:	ASN ND2	122	-26.65	-26.65	27.33
ASN C	122	-28.42	-42.42	25.04	:	ASN O	122	-29.52	-29.52	25.43
ARG N	123	-27.98	-43.66	25.22	:	ARG CA	123	-28.84	-28.84	25.72
ARG CB	123	-28.18	-45.97	25.51	:	ARG CG	123	-26.78	-26.78	26.17
ARG CD	123	-26.34	-46.96	27.34	:	ARG NE	123	-26.83	-26.83	28.73

9/32

III 1.9.

ARG CZ	123	-27.92	-47.53	29.20	:	ARG NH1	123	-28.26	-28.26	30.51
ARG NH2	123	-28.69	-48.33	28.35	:	ARG C	123	-29.16	-29.16	27.17
ARG O	123	-29.99	-45.29	27.68	:	ASP N	124	-28.41	-28.41	27.89
ASP CA	124	-28.41	-43.82	29.32	:	ASP CB	124	-27.00	-27.00	29.66
ASP CG	124	-26.82	-43.92	31.10	:	ASP OD1	124	-27.09	-27.09	31.98
ASP OD2	124	-26.50	-45.09	31.31	:	ASP C	124	-29.33	-29.33	29.92
ASP O	124	-29.39	-41.67	29.34	:	PRO N	125	-30.06	-30.06	31.04
PRO CD	125	-30.08	-44.21	31.82	:	PRO CA	125	-31.11	-31.11	31.51
PRO CB	125	-32.18	-43.01	31.95	:	PRO CG	125	-31.31	-31.31	32.70
PRO C	125	-30.60	-41.19	32.61	:	PRO O	125	-31.38	-31.38	33.15
LYS N	126	-29.29	-41.29	32.93	:	LYS CA	126	-28.78	-28.78	33.91
LYS CB	126	-28.84	-41.09	35.28	:	LYS CG	126	-27.64	-27.64	36.08
LYS CD	126	-26.81	-42.73	35.39	:	LYS CE	126	-25.85	-25.85	36.36
LYS NZ	126	-25.25	-42.56	37.35	:	LYS C	126	-27.42	-27.42	33.54
LYS O	126	-27.33	-38.50	33.61	:	GLU N	127	-26.40	-26.40	33.07
GLU CA	127	-25.14	-39.81	32.71	:	GLU CB	127	-24.13	-24.13	32.94
GLU CG	127	-23.20	-40.68	34.17	:	GLU CD	127	-23.80	-23.80	35.61
GLU OE1	127	-24.84	-39.90	35.86	:	GLU OE2	127	-23.27	-23.27	36.56
GLU C	127	-25.15	-39.17	31.28	:	GLU O	127	-25.88	-25.88	30.39
ASP N	128	-24.51	-38.01	30.97	:	ASP CA	128	-24.42	-24.42	29.59
ASP CB	128	-23.82	-36.04	29.56	:	ASP CG	128	-24.72	-24.72	30.18
ASP OD1	128	-24.75	-33.82	29.78	:	ASP OD2	128	-25.42	-25.42	31.15
ASP C	128	-23.55	-38.30	28.66	:	ASP O	128	-22.91	-22.91	29.09
LEU N	129	-23.48	-37.96	27.37	:	LEU CA	129	-22.63	-22.63	26.39
LEU CB	129	-23.33	-38.90	25.07	:	LEU CG	129	-22.98	-22.98	24.13
LEU CD1	129	-23.13	-39.52	22.75	:	LEU CD2	129	-21.59	-21.59	24.30
LEU C	129	-21.54	-37.63	26.09	:	LEU O	129	-21.95	-21.95	25.88
ARG N	130	-20.24	-37.98	26.09	:	ARG CA	130	-19.26	-19.26	25.66
ARG CB	130	-18.44	-36.57	26.87	:	ARG CG	130	-19.22	-19.22	27.86
ARG CD	130	-18.43	-34.73	28.70	:	ARG NE	130	-17.26	-17.26	29.25
ARG CZ	130	-16.05	-34.80	29.39	:	ARG NH1	130	-15.10	-15.10	29.95
ARG NH2	130	-15.64	-33.58	28.94	:	ARG C	130	-18.36	-18.36	24.52
ARG O	130	-17.39	-38.20	24.75	:	ILE N	131	-18.52	-18.52	23.24
ILE CA	131	-17.68	-37.73	22.17	:	ILE CB	131	-18.61	-18.61	20.99
ILE CG2	131	-17.86	-38.40	19.73	:	ILE CG1	131	-19.50	-19.50	21.44
ILE CD1	131	-20.52	-39.68	20.45	:	ILE C	131	-16.58	-16.58	21.79
ILE O	131	-16.80	-35.58	21.98	:	ILE N	132	-15.42	-15.42	21.31
ILE CA	132	-14.31	-36.36	20.82	:	ILE CB	132	-13.06	-13.06	21.79
ILE CG2	132	-12.38	-37.80	21.79	:	ILE CG1	132	-11.95	-11.95	21.26
ILE CD1	132	-12.16	-34.09	21.44	:	ILE C	132	-14.02	-14.02	19.44
ILE O	132	-14.06	-38.21	19.37	:	GLN N	133	-13.77	-13.77	18.28
GLN CA	133	-13.61	-37.13	17.05	:	GLN CB	133	-14.76	-14.76	16.13
GLN CG	133	-16.08	-37.06	16.81	:	GLN CD	133	-17.25	-17.25	15.86
GLN OE1	133	-17.14	-37.00	14.66	:	GLN NE2	133	-18.47	-18.47	16.28
GLN C	133	-12.46	-36.54	16.31	:	GLN O	133	-12.25	-12.25	16.42
LEU N	134	-11.69	-37.35	15.61	:	LEU CA	134	-10.65	-10.65	14.76
LEU CB	134	-9.42	-37.67	14.78	:	LEU CG	134	-8.39	-8.39	13.77
LEU CD1	134	-7.62	-36.10	14.11	:	LEU CD2	134	-7.47	-7.47	13.73
LEU C	134	-11.35	-36.91	13.42	:	LEU O	134	-11.86	-11.86	13.10
ALA N	135	-11.48	-35.87	12.63	:	ALA CA	135	-12.19	-12.19	11.40
ALA CB	135	-13.27	-34.89	11.39	:	ALA C	135	-11.15	-11.15	10.34
ALA O	135	-10.30	-34.77	10.58	:	MET N	136	-11.13	-11.13	9.19
MET CA	136	-10.17	-36.01	8.14	:	MET CB	136	-9.42	-9.42	7.85
MET CG	136	-8.72	-37.84	9.12	:	MET SD	136	-8.72	-8.72	9.74
MET CE	136	-10.20	-39.92	10.67	:	MET C	136	-11.01	-11.01	6.95
MET O	136	-11.64	-36.43	6.36	:	PRO N	137	-11.22	-11.22	6.55
PRO CD	137	-10.68	-33.11	7.14	:	PRO CA	137	-12.14	-12.14	5.49
PRO CB	137	-12.24	-32.44	5.61	:	PRO CG	137	-11.86	-11.86	7.02
PRO C	137	-11.66	-34.38	4.13	:	PRO O	137	-10.47	-10.47	3.85

10/32

III 1-10.

VAL N	138	-12.58	-34.81	3.28	:	VAL CA	138	-12.31	-12.31	1.95
VAL CB	138	-13.48	-36.17	1.52	:	VAL CG1	138	-13.40	-13.40	0.11
VAL CG2	138	-13.41	-37.40	2.33	:	VAL C	138	-12.06	-12.06	0.94
VAL O	138	-11.28	-34.37	0.02	:	ASN N	139	-12.78	-12.78	1.02
ASN CA	139	-12.74	-31.94	0.07	:	ASN CB	139	-14.11	-14.11	0.03
ASN CG	139	-15.11	-32.24	-0.64	:	ASN OD1	139	-16.26	-16.26	-0.25
ASN ND2	139	-14.75	-32.85	-1.75	:	ASN C	139	-11.75	-11.75	0.09
ASN O	139	-11.19	-30.37	-0.93	:	ASN N	140	-11.61	-11.61	1.24
ASN CA	140	-10.74	-29.01	1.55	:	ASN CB	140	-11.22	-11.22	0.98
ASN CG	140	-12.71	-27.61	1.05	:	ASN OD1	140	-13.29	-13.29	2.06
ASN ND2	140	-13.44	-27.87	0.00	:	ASN C	140	-10.77	-10.77	3.04
ASN O	140	-11.72	-29.44	3.54	:	FRO N	141	-9.98	-9.98	3.90
PRO CD	141	-8.90	-27.39	3.54	:	PRO CA	141	-9.86	-9.86	5.32
PRO CB	141	-8.61	-27.99	5.78	:	PRO CG	141	-8.55	-8.55	4.89
PRO C	141	-11.01	-28.39	6.27	:	PRO O	141	-10.91	-10.91	7.49
GLN N	142	-12.13	-27.94	5.73	:	GLN CA	142	-13.34	-13.34	6.45
GLN CB	142	-14.15	-26.64	5.77	:	GLN CG	142	-13.23	-13.23	5.02
GLN CD	142	-13.43	-24.42	5.61	:	GLN OE1	142	-14.56	-14.56	5.48
GLN NE2	142	-12.42	-23.91	6.35	:	GLN C	142	-14.21	-14.21	6.46
GLN O	142	-14.32	-29.46	5.42	:	ILE N	143	-14.88	-14.88	7.56
ILE CA	143	-15.73	-30.31	7.60	:	ILE CB	143	-15.46	-15.46	8.92
ILE CG2	143	-15.41	-30.26	10.15	:	ILE CG1	143	-16.57	-16.57	9.05
ILE CD1	143	-16.22	-33.21	10.01	:	ILE C	143	-17.14	-17.14	7.48
ILE O	143	-17.39	-28.61	7.99	:	HIS N	144	-18.00	-18.00	6.68
HIS CA	144	-19.34	-29.88	6.45	:	HIS CB	144	-19.58	-19.58	4.99
HIS CG	144	-18.53	-28.73	4.36	:	HIS CD2	144	-17.86	-17.86	3.31
HIS ND1	144	-18.00	-27.57	4.68	:	HIS CE1	144	-17.01	-17.01	3.88
HIS NE2	144	-16.95	-28.35	3.06	:	HIS C	144	-20.32	-20.32	6.87
HIS O	144	-20.12	-32.15	6.57	:	GLU N	145	-21.40	-21.40	7.54
GLU CA	145	-22.39	-31.56	7.97	:	GLU CB	145	-22.62	-22.62	9.36
GLU CG	145	-21.61	-32.31	9.92	:	GLU CD	145	-21.37	-21.37	11.38
GLU OE1	145	-20.21	-32.02	11.80	:	GLU OE2	145	-22.34	-22.34	12.11
GLU C	145	-23.67	-31.35	7.24	:	GLU O	145	-24.26	-24.26	7.25
PHE N	146	-24.10	-32.39	6.57	:	PHE CA	146	-25.31	-25.31	5.83
PHE CB	146	-25.09	-32.99	4.51	:	PHE CG	146	-24.19	-24.19	3.54
PHE CD1	146	-22.83	-32.34	3.63	:	PHE CD2	146	-24.76	-24.76	2.60
PHE CE1	146	-22.04	-31.65	2.77	:	PHE CE2	146	-23.96	-23.96	1.75
PHE CZ	146	-22.61	-30.85	1.83	:	PHE C	146	-26.38	-26.38	6.67
PHE O	146	-26.43	-34.16	6.66	:	PHE N	147	-27.24	-27.24	7.41
PHE CA	147	-28.25	-32.85	8.20	:	PHE CB	147	-28.77	-28.77	9.28
PHE CG	147	-27.96	-32.05	10.55	:	PHE CD1	147	-27.09	-27.09	10.91
PHE CD2	147	-28.03	-33.19	11.31	:	PHE CE1	147	-26.30	-26.30	12.03
PHE CE2	147	-27.23	-33.35	12.42	:	PHE CZ	147	-26.36	-26.36	12.78
PHE C	147	-29.38	-33.14	7.26	:	PHE O	147	-29.72	-29.72	6.46
LEU N	148	-29.97	-34.33	7.29	:	LEU CA	148	-31.14	-31.14	6.48
LEU CB	148	-31.49	-36.11	6.51	:	LEU CG	148	-31.58	-31.58	5.26
LEU CD1	148	-32.43	-38.14	5.53	:	LEU CD2	148	-32.29	-32.29	4.19
LEU C	148	-32.38	-33.95	7.01	:	LEU O	148	-33.33	-33.33	6.24
SER N	149	-32.37	-33.56	8.29	:	SER CA	149	-33.58	-33.58	8.92
SER CB	149	-33.30	-33.21	10.40	:	SER OG	149	-32.18	-32.18	10.87
SER C	149	-34.53	-31.98	8.70	:	SER O	149	-35.63	-35.63	8.79
SER N	150	-34.58	-30.69	8.39	:	SER CA	150	-35.84	-35.84	8.54
SER CB	150	-37.05	-30.34	7.76	:	SER OG	150	-37.23	-37.23	6.81
SER C	150	-36.32	-29.80	10.00	:	SER O	150	-36.99	-36.99	10.59
THR N	151	-35.99	-28.67	10.62	:	THR CA	151	-36.11	-36.11	12.06
THR CB	151	-34.87	-28.95	12.85	:	THR OG1	151	-33.85	-33.85	12.10
THR CG2	151	-34.74	-30.43	13.15	:	THR C	151	-36.46	-36.46	12.72
THR O	151	-37.00	-27.46	13.80	:	GLU N	152	-36.27	-36.27	12.07
GLU CA	152	-36.43	-24.83	12.73	:	GLU CB	152	-37.92	-37.92	13.18

11/32

III - 11.

GLU CG 152	-38.53	-25.06	14.54	:	GLU CD 152	-38.34	-38.34	15.68
GLU OE1 152	-38.86	-24.28	16.80	:	GLU OE2 152	-37.74	-37.74	15.41
GLU C 152	-35.43	-24.88	13.88	:	GLU O 152	-35.53	-35.53	14.96
ALA N 153	-34.29	-24.55	13.27	:	ALA CA 153	-32.93	-32.93	13.81
ALA CB 153	-32.52	-25.77	14.62	:	ALA C 153	-32.18	-32.18	12.52
ALA O 153	-31.36	-23.84	12.22	:	GLN N 154	-32.53	-32.53	11.68
GLN CA 154	-31.77	-25.92	10.51	:	GLN CB 154	-30.63	-30.63	11.02
GLN CG 154	-30.97	-28.24	11.41	:	GLN CD 154	-31.29	-31.29	10.12
GLN OE1 154	-32.46	-29.28	9.86	:	GLN NE2 154	-30.33	-30.33	9.20
GLN C 154	-32.29	-26.35	9.15	:	GLN O 154	-31.39	-31.39	8.34
GLN N 155	-33.50	-26.68	8.69	:	GLN CA 155	-33.76	-33.76	7.22
GLN CB 155	-33.41	-25.57	6.45	:	GLN CG 155	-33.48	-33.48	4.93
GLN CD 155	-34.59	-24.56	4.35	:	GLN OE1 155	-35.54	-35.54	5.03
GLN NE2 155	-34.53	-24.23	3.04	:	GLN C 155	-33.11	-33.11	6.47
GLN O 155	-31.92	-28.10	6.31	:	SER N 156	-33.85	-33.85	5.98
SER CA 156	-33.32	-30.25	5.33	:	SER CB 156	-34.46	-34.46	4.97
SER OG 156	-34.05	-32.24	4.10	:	SER C 156	-32.58	-32.58	4.06
SER O 156	-33.19	-29.19	3.24	:	TYR N 157	-31.37	-31.37	3.75
TYR CA 157	-30.76	-30.07	2.49	:	TYR CB 157	-29.40	-29.40	2.33
TYR CG 157	-29.27	-32.19	2.37	:	TYR CD1 157	-28.82	-28.82	3.49
TYR CE1 157	-28.72	-34.17	3.53	:	TYR CD2 157	-29.61	-29.61	1.27
TYR CE2 157	-29.51	-34.25	1.30	:	TYR CZ 157	-29.07	-29.07	2.42
TYR OH 157	-29.03	-36.25	2.43	:	TYR C 157	-31.63	-31.63	1.30
TYR O 157	-31.46	-29.87	0.24	:	LEU N 158	-32.64	-32.64	1.42
LEU CA 158	-33.60	-31.62	0.34	:	LEU CB 158	-34.71	-34.71	0.75
LEU CG 158	-34.74	-34.06	0.44	:	LEU CD1 158	-33.92	-33.92	-0.79
LEU CD2 158	-34.18	-34.87	1.58	:	LEU C 158	-34.32	-34.32	-0.11
LEU O 158	-34.67	-30.20	-1.28	:	GLN N 159	-34.53	-34.53	0.79
GLN CA 159	-35.19	-28.14	0.45	:	GLN CB 159	-35.47	-35.47	1.68
GLN CG 159	-36.42	-28.08	2.55	:	GLN CD 159	-36.61	-36.61	3.91
GLN OE1 159	-36.07	-27.90	4.93	:	GLN NE2 159	-37.44	-37.44	3.94
GLN C 159	-34.41	-27.27	-0.51	:	GLN O 159	-35.04	-35.04	-0.99
GLU N 160	-33.14	-27.46	-0.84	:	GLU CA 160	-32.50	-32.50	-1.76
GLU CB 160	-31.04	-26.48	-1.45	:	GLU CG 160	-30.73	-30.73	-0.11
GLU CD 160	-31.52	-24.58	0.25	:	GLU OE1 160	-32.00	-32.00	1.40
GLU OE2 160	-31.65	-23.66	-0.59	:	GLU C 160	-32.67	-32.67	-3.23
GLU O 160	-32.28	-26.13	-4.15	:	PHE N 161	-33.23	-33.23	-3.47
PHE CA 161	-33.52	-28.52	-4.81	:	PHE CB 161	-33.79	-33.79	-4.78
PHE CG 161	-32.49	-30.74	-4.67	:	PHE CD1 161	-32.25	-32.25	-3.56
PHE CD2 161	-31.58	-30.60	-5.67	:	PHE CE1 161	-31.05	-31.05	-3.45
PHE CE2 161	-30.39	-31.25	-5.56	:	PHE CZ 161	-30.14	-30.14	-4.45
PHE C 161	-34.73	-27.77	-5.30	:	PHE O 161	-35.53	-35.53	-4.50
SER N 162	-34.89	-27.59	-6.60	:	SER GA 162	-35.97	-35.97	-7.03
SER CB 162	-35.61	-26.30	-8.44	:	SER OG 162	-35.27	-35.27	-9.16
SER C 162	-37.31	-27.46	-6.94	:	SER O 162	-37.35	-37.35	-6.63
LYS N 163	-38.45	-26.84	-7.21	:	LYS CA 163	-39.72	-39.72	-6.99
LYS CB 163	-40.84	-26.56	-7.22	:	LYS CG 163	-41.94	-41.94	-6.24
LYS CD 163	-43.08	-25.68	-6.74	:	LYS CE 163	-43.78	-43.78	-8.06
LYS NZ 163	-44.10	-27.66	-8.04	:	LYS C 163	-39.90	-39.90	-7.95
LYS O 163	-40.17	-29.76	-7.52	:	HIS N 164	-39.73	-39.73	-9.25
HIS CA 164	-39.92	-29.49	-10.23	:	HIS CB 164	-39.64	-39.64	-11.68
HIS CG 164	-39.24	-30.07	-12.73	:	HIS CD2 164	-39.59	-39.59	-14.10
HIS ND1 164	-38.45	-31.19	-12.61	:	HIS CE1 164	-38.32	-38.32	-13.78
HIS NE2 164	-39.01	-31.07	-14.68	:	HIS C 164	-38.99	-38.99	-9.92
HIS O 164	-39.39	-31.79	-10.14	:	ILE N 165	-37.72	-37.72	-9.55
ILE CA 165	-36.87	-31.57	-9.33	:	ILE CB 165	-35.45	-35.45	-9.14
ILE CG2 165	-34.53	-31.98	-8.41	:	ILE CG1 165	-35.02	-35.02	-10.55
ILE CD1 165	-33.58	-30.40	-10.81	:	ILE C 165	-37.40	-37.40	-8.15
ILE O 165	-37.41	-33.62	-8.28	:	LEU N 166	-37.98	-37.98	-7.11

12/32

III - 1.12

LEU CA	166	-38.48	-32.52	-5.97	:	LEU CB	166	-38.75	-38.75	-4.84
LEU CG	166	-37.87	-31.47	-3.61	:	LEU CD1	166	-36.66	-36.66	-3.74
LEU CD2	166	-37.41	-30.07	-3.44	:	LEU C	166	-39.74	-39.74	-6.38
LEU O	166	-39.85	-34.47	-6.15	:	GLU N	167	-40.65	-40.65	-7.09
GLU CA	167	-41.88	-33.22	-7.51	:	GLU CB	167	-42.78	-42.78	-8.24
GLU CG	167	-43.37	-31.11	-7.44	:	GLU CD	167	-44.52	-44.52	-8.19
GLU OE1	167	-44.47	-30.18	-9.38	:	GLU OE2	167	-45.55	-45.55	-7.60
GLU C	167	-41.59	-34.41	-8.44	:	GLU O	167	-42.08	-42.08	-8.22
ALA N	168	-40.67	-34.28	-9.38	:	ALA CA	168	-40.46	-40.46	-10.34
ALA CB	168	-39.68	-34.79	-11.48	:	ALA C	168	-39.72	-39.72	-9.65
ALA O	168	-40.04	-37.62	-9.85	:	SER N	169	-38.77	-38.77	-8.78
SER CA	169	-38.10	-37.14	-7.99	:	SER CB	169	-37.07	-37.07	-7.08
SER OG	169	-36.02	-35.94	-7.82	:	SER C	169	-39.05	-39.05	-7.11
SER O	169	-39.19	-39.13	-7.32	:	PHE N	170	-39.72	-39.72	-6.14
PHE CA	170	-40.60	-38.05	-5.25	:	PHE CB	170	-40.81	-40.81	-3.95
PHE CG	170	-39.54	-37.04	-3.13	:	PHE CD1	170	-38.85	-38.85	-2.68
PHE CD2	170	-39.05	-35.79	-2.91	:	PHE CE1	170	-37.67	-37.67	-2.01
PHE CE2	170	-37.86	-35.62	-2.24	:	PHE CZ	170	-37.17	-37.17	-1.80
PHE C	170	-41.93	-38.40	-5.87	:	PHE O	170	-42.70	-42.70	-5.20
ASN N	171	-42.20	-37.98	-7.15	:	ASN CA	171	-43.44	-43.44	-7.90
ASN CB	171	-43.57	-39.73	-8.24	:	ASN CG	171	-44.74	-44.74	-9.18
ASN OD1	171	-45.26	-39.16	-9.87	:	ASN ND2	171	-45.21	-45.21	-9.32
ASN C	171	-44.62	-37.83	-7.04	:	ASN O	171	-45.26	-45.26	-6.40
SER N	172	-44.83	-36.55	-6.83	:	SER CA	172	-45.90	-45.90	-5.98
SER CB	172	-45.57	-36.23	-4.50	:	SER OG	172	-45.71	-45.71	-3.99
SER C	172	-46.11	-34.56	-6.24	:	SER O	172	-45.29	-45.29	-6.91
LYS N	173	-47.28	-34.04	-5.85	:	LYS CA	173	-47.49	-47.49	-6.01
LYS CB	173	-48.99	-32.46	-6.05	:	LYS CG	173	-49.45	-49.45	-7.51
LYS CD	173	-48.84	-31.14	-8.27	:	LYS CE	173	-48.12	-48.12	-9.70
LYS NZ	173	-46.79	-32.04	-9.69	:	LYS C	173	-46.74	-46.74	-4.89
LYS O	173	-46.52	-32.54	-3.83	:	PHE N	174	-46.22	-46.22	-5.17
PHE CA	174	-45.24	-30.19	-4.25	:	PHE CB	174	-44.62	-44.62	-4.82
PHE CG	174	-43.66	-28.22	-3.79	:	PHE CD1	174	-42.48	-42.48	-3.41
PHE CD2	174	-44.03	-27.09	-3.08	:	PHE CE1	174	-41.73	-41.73	-2.34
PHE CE2	174	-43.29	-26.63	-2.02	:	PHE CZ	174	-42.14	-42.14	-1.65
PHE C	174	-45.80	-29.98	-2.84	:	PHE O	174	-45.15	-45.15	-1.85
GLU N	175	-46.96	-29.41	-2.74	:	GLU CA	175	-47.58	-47.58	-1.48
GLU CB	175	-48.89	-28.45	-1.62	:	GLU CG	175	-50.07	-50.07	-2.47
GLU CD	175	-49.50	-29.57	-3.75	:	GLU OE1	175	-49.33	-49.33	-3.67
GLU OE2	175	-49.07	-28.86	-4.71	:	GLU C	175	-47.78	-47.78	-0.88
GLU O	175	-47.70	-30.65	0.34	:	GLU N	176	-47.91	-47.91	-1.48
GLU CA	176	-47.95	-33.04	-0.68	:	GLU CB	176	-48.39	-48.39	-1.56
GLU CG	176	-48.15	-35.69	-1.26	:	GLU CD	176	-48.70	-48.70	0.07
GLU OE1	176	-49.05	-35.53	1.02	:	GLU OE2	176	-48.73	-48.73	0.14
GLU C	176	-46.56	-33.27	-0.05	:	GLU O	176	-46.47	-46.47	1.19
ILE N	177	-45.47	-33.25	-0.86	:	ILE CA	177	-44.04	-44.04	-0.46
ILE CB	177	-43.04	-33.02	-1.60	:	ILE CG2	177	-41.64	-41.64	-1.10
ILE CG1	177	-42.95	-34.20	-2.52	:	ILE CD1	177	-42.17	-42.17	-3.84
ILE C	177	-43.76	-32.42	0.67	:	ILE O	177	-43.05	-43.05	1.61
ASN N	178	-44.28	-31.22	0.68	:	ASN CA	178	-43.94	-43.94	1.71
ASN CB	178	-44.32	-28.95	1.15	:	ASN CG	178	-43.69	-43.69	1.96
ASN OD1	178	-43.06	-26.95	1.36	:	ASN ND2	178	-43.77	-43.77	3.30
ASN C	178	-44.63	-30.59	3.07	:	ASN O	178	-44.02	-44.02	4.14
ARG N	179	-45.93	-30.90	3.05	:	ARG CA	179	-46.74	-46.74	4.23
ARG CB	179	-48.20	-31.51	3.86	:	ARG CG	179	-49.14	-49.14	4.89
ARG CD	179	-50.28	-32.84	4.05	:	ARG NE	179	-50.02	-50.02	3.53
ARG CZ	179	-49.94	-35.31	4.35	:	ARG NH1	179	-49.70	-49.70	3.82
ARG NH2	179	-50.05	-35.12	5.70	:	ARG C	179	-46.15	-46.15	4.82
ARG O	179	-45.87	-32.43	6.01	:	VAL N	180	-45.89	-45.89	4.03

13/32

III. 1.13.

VAL CA	180	-45.38	-34.66	4.73	:	VAL CB	180	-45.76	-45.76	3.89
VAL CG1	180	-45.60	-35.78	2.39	:	VAL CG2	180	-44.82	-44.82	4.29
VAL C	180	-43.89	-34.57	5.13	:	VAL O	180	-43.55	-43.55	6.21
LEU N	181	-42.99	-33.92	4.36	:	LEU CA	181	-41.53	-41.53	4.64
LEU CB	181	-40.79	-33.84	3.34	:	LEU CG	181	-39.78	-39.78	3.09
LEU CD1	181	-40.23	-36.27	3.52	:	LEU CD2	181	-39.50	-39.50	1.60
LEU C	181	-40.99	-32.51	5.36	:	LEU O	181	-40.01	-40.01	6.08
PHE N	182	-41.55	-31.34	5.15	:	PHE CA	182	-40.95	-40.95	5.61
PHE CB	182	-40.31	-29.33	4.46	:	PHE CG	182	-39.44	-39.44	3.49
PHE CD1	182	-38.40	-30.89	3.94	:	PHE CD2	182	-39.73	-39.73	2.15
PHE CE1	182	-37.66	-31.60	3.04	:	PHE CE2	182	-38.98	-38.98	1.26
PHE CZ	182	-37.95	-31.53	1.70	:	PHE C	182	-41.98	-41.98	6.23
PHE O	182	-41.68	-27.96	6.39	:	GLU N	183	-43.21	-43.21	6.58
GLU CA	183	-44.16	-28.56	7.08	:	GLU CB	183	-45.55	-45.55	7.01
GLU CG	183	-46.88	-28.39	7.04	:	GLU CD	183	-48.14	-48.14	7.08
GLU OE1	183	-48.11	-30.36	7.91	:	GLU OE2	183	-49.13	-49.13	6.28
GLU C	183	-43.73	-28.16	8.52	:	GLU O	183	-43.31	-43.31	9.40
GLU N	184	-43.76	-26.81	8.57	:	GLU CA	184	-43.26	-43.26	9.65
GLU CB	184	-43.51	-24.46	9.22	:	GLU CG	184	-42.95	-42.95	10.10
GLU CD	184	-44.00	-22.66	11.05	:	GLU OE1	184	-44.07	-44.07	11.05
GLU OE2	184	-44.76	-23.39	11.77	:	GLU C	184	-43.79	-43.79	11.02
GLU O	184	-42.96	-26.41	11.92	:	GLU N	185	-45.08	-45.08	11.30
GLU CA	185	-45.43	-26.70	12.65	:	GLU CB	185	-46.90	-46.90	13.08
GLU CG	185	-46.99	-26.66	14.64	:	GLU CD	185	-45.94	-45.94	15.47
GLU OE1	185	-44.76	-26.28	15.58	:	GLU OE2	185	-46.35	-46.35	16.00
GLU C	185	-45.25	-28.21	12.60	:	GLU O	185	-45.30	-45.30	11.50
GLY N	186	-45.01	-28.94	13.67	:	GLY CA	186	-44.73	-44.73	13.46
GLY C	186	-43.27	-30.58	13.06	:	GLY O	186	-42.78	-42.78	13.16
GLN N	187	-42.57	-29.50	12.62	:	GLN CA	187	-41.12	-41.12	12.52
GLN CB	187	-40.50	-28.24	12.16	:	GLN CG	187	-40.31	-40.31	10.69
GLN CD	187	-39.52	-26.85	10.63	:	GLN OE1	187	-38.30	-38.30	10.37
GLN NE2	187	-40.12	-25.69	10.96	:	GLN C	187	-40.64	-40.64	13.93
GLN O	187	-41.39	-29.59	14.91	:	GLN N	188	-39.35	-39.35	14.08
GLN CA	188	-38.95	-30.45	15.36	:	GLN CB	188	-38.47	-38.47	14.97
GLN CG	188	-37.95	-32.96	15.92	:	GLN CD	188	-38.88	-38.88	17.09
GLN OE1	188	-39.62	-34.07	17.25	:	GLN NE2	188	-38.86	-38.86	18.00
GLN C	188	-37.99	-29.54	16.09	:	GLN O	188	-37.27	-37.27	16.85
GLU N	189	-37.78	-28.23	16.04	:	GLU CA	189	-36.82	-36.82	16.92
GLU CB	189	-37.18	-27.67	18.44	:	GLU CG	189	-38.04	-38.04	18.86
GLU CD	189	-38.38	-26.37	20.37	:	GLU OE1	189	-39.57	-39.57	20.73
GLU OE2	189	-37.47	-25.97	21.18	:	GLU C	189	-35.32	-35.32	16.84
GLU O	189	-34.54	-27.00	17.38	:	GLY N	190	-34.76	-34.76	16.25
GLY CA	190	-33.31	-28.93	16.30	:	GLY C	190	-32.80	-32.80	16.19
GLY O	190	-33.56	-31.26	16.36	:	VAL N	191	-31.52	-31.52	15.94
VAL CA	191	-30.98	-31.72	15.64	:	VAL CB	191	-29.79	-29.79	14.73
VAL CG1	191	-30.23	-30.73	13.55	:	VAL CG2	191	-28.70	-28.70	15.34
VAL C	191	-30.61	-32.61	16.79	:	VAL O	191	-30.10	-30.10	16.51
ILE N	192	-30.73	-32.32	18.08	:	ILE CA	192	-30.34	-30.34	19.14
ILE CB	192	-29.21	-32.72	20.03	:	ILE CG2	192	-29.09	-29.09	21.14
ILE CG1	192	-27.85	-32.61	19.35	:	ILE CD1	192	-26.85	-26.85	20.05
ILE C	192	-31.65	-33.12	19.86	:	ILE O	192	-31.93	-31.93	20.50
VAL N	193	-32.49	-34.08	19.52	:	VAL CA	193	-33.88	-33.88	19.95
VAL CB	193	-34.67	-34.82	18.79	:	VAL CG1	193	-35.79	-35.79	19.25
VAL CG2	193	-35.32	-33.72	18.02	:	VAL C	193	-33.82	-33.82	21.13
VAL O	193	-33.00	-36.07	21.05	:	ASN N	194	-34.61	-34.61	22.19
ASN CA	194	-34.53	-36.17	23.13	:	ASN CB	194	-34.64	-34.64	24.57
ASN CG	194	-35.99	-35.21	24.89	:	ASN OD1	194	-36.50	-36.50	24.14
ASN ND2	194	-36.52	-35.72	26.01	:	ASN C	194	-35.74	-35.74	22.82
ASN O	194	-36.82	-36.56	22.44	:	ILE N	195	-35.47	-35.47	22.91

14/32

III 14

ILE CA 195	-36.53	-39.25	22.68	:	ILE CB 195	-36.12	-36.12	21.69
ILE CG2 195	-36.41	-39.57	20.41	:	ILE CG1 195	-34.73	-34.73	21.79
ILE CD1 195	-34.46	-41.71	23.06	:	ILE C 195	-36.83	-36.83	24.03
ILE O 195	-36.34	-39.35	25.07	:	ASP N 196	-37.63	-37.63	24.03
ASP CA 196	-37.98	-41.53	25.27	:	ASP CB 196	-39.52	-39.52	25.40
ASP CG 196	-40.08	-42.81	25.97	:	ASP OD1 196	-40.21	-40.21	27.21
ASP OD2 196	-40.21	-43.76	25.15	:	ASP C 196	-37.43	-37.43	25.38
ASP O 196	-37.40	-43.83	24.50	:	SER N 197	-37.22	-37.22	26.67
SER CA 197	-36.86	-44.22	27.41	:	SER CB 197	-37.51	-37.51	28.78
SER OG 197	-37.60	-42.68	29.18	:	SER C 197	-37.28	-37.28	26.73
SER O 197	-36.40	-46.33	26.38	:	GLU N 198	-38.60	-38.60	26.48
GLU CA 198	-39.08	-46.78	25.81	:	GLU CB 198	-40.60	-40.60	25.64
GLU CG 198	-41.35	-46.78	27.01	:	GLU CD 198	-42.11	-42.11	27.37
GLU OE1 198	-41.91	-44.98	28.52	:	GLU OE2 198	-42.90	-42.90	26.48
GLU C 198	-38.45	-47.06	24.42	:	GLU O 198	-37.90	-37.90	24.27
GLN N 199	-38.43	-46.12	23.43	:	GLN CA 199	-37.81	-37.81	22.13
GLN CB 199	-37.74	-45.11	21.28	:	GLN CG 199	-39.11	-39.11	20.94
GLN CD 199	-39.18	-42.89	20.83	:	GLN OE1 199	-38.88	-38.88	21.83
GLN NE2 199	-39.59	-42.26	19.71	:	GLN C 199	-36.38	-36.38	22.25
GLN O 199	-36.07	-48.15	21.75	:	ILE N 200	-35.52	-35.52	23.06
ILE CA 200	-34.13	-46.81	23.22	:	ILE CB 200	-33.47	-33.47	24.42
ILE CG2 200	-31.99	-46.51	24.49	:	ILE CG1 200	-33.68	-33.68	24.33
ILE CD1 200	-33.59	-43.99	25.72	:	ILE C 200	-33.96	-33.96	23.44
ILE O 200	-33.10	-48.96	22.80	:	LYS N 201	-34.83	-34.83	24.34
LYS CA 201	-34.70	-50.22	24.82	:	LYS CB 201	-35.92	-35.92	25.67
LYS CG 201	-35.62	-52.09	26.34	:	LYS CD 201	-36.83	-36.83	27.05
LYS CE 201	-36.35	-53.82	28.11	:	LYS NZ 201	-37.41	-37.41	29.00
LYS C 201	-34.53	-51.28	23.74	:	LYS O 201	-33.53	-33.53	23.78
GLU N 202	-35.49	-51.25	22.78	:	GLU CA 202	-35.47	-35.47	21.89
GLU CB 202	-36.76	-52.38	21.01	:	GLU CG 202	-37.04	-37.04	20.13
GLU CD 202	-36.64	-55.03	20.75	:	GLU OE1 202	-35.44	-35.44	20.69
GLU OE2 202	-37.47	-55.63	21.48	:	GLU C 202	-34.15	-34.15	21.09
GLU O 202	-33.33	-53.26	21.13	:	LEU N 203	-33.88	-33.88	20.68
LEU CA 203	-32.64	-50.63	19.98	:	LEU CB 203	-32.68	-32.68	19.63
LEU CG 203	-31.99	-48.42	18.48	:	LEU CD1 203	-31.37	-31.37	19.00
LEU CD2 203	-30.92	-49.27	17.86	:	LEU C 203	-31.39	-31.39	20.84
LEU O 203	-30.42	-51.45	20.23	:	SER N 204	-31.33	-31.33	22.20
SER CA 204	-30.06	-50.93	22.91	:	SER CB 204	-30.09	-30.09	24.36
SER OG 204	-30.72	-49.47	24.62	:	SER C 204	-29.61	-29.61	22.83
SER O 204	-28.43	-52.69	22.61	:	LYS N 205	-30.67	-30.67	23.01
LYS CA 205	-30.57	-54.59	23.03	:	LYS CB 205	-31.98	-31.98	23.07
LYS CG 205	-32.16	-56.55	23.41	:	LYS CD 205	-33.66	-33.66	23.17
LYS CE 205	-34.57	-55.86	24.09	:	LYS NZ 205	-35.57	-35.57	23.29
LYS C 205	-29.80	-55.13	21.83	:	LYS O 205	-28.68	-28.68	21.92
HIS N 206	-30.44	-54.82	20.69	:	HIS CA 206	-29.90	-29.90	19.40
HIS CB 206	-30.87	-54.72	18.31	:	HIS CG 206	-30.37	-30.37	16.97
HIS CD2 206	-30.02	-56.52	16.69	:	HIS ND1 206	-30.07	-30.07	15.89
HIS CE1 206	-29.55	-55.30	14.97	:	HIS NE2 206	-29.52	-29.52	15.47
HIS C 206	-28.46	-54.70	19.19	:	HIS O 206	-27.62	-27.62	18.82
ALA N 207	-28.16	-53.42	19.47	:	ALA CA 207	-26.81	-26.81	19.35
ALA CB 207	-26.83	-51.46	19.86	:	ALA C 207	-25.76	-25.76	20.12
ALA O 207	-24.74	-54.22	19.60	:	LYS N 208	-26.10	-26.10	21.40
LYS CA 208	-25.19	-54.66	22.33	:	LYS CB 208	-25.85	-25.85	23.68
LYS CG 208	-25.67	-53.54	24.54	:	LYS CD 208	-26.66	-26.66	25.65
LYS CE 208	-26.62	-52.92	26.82	:	LYS NZ 208	-25.33	-25.33	27.46
LYS C 208	-24.74	-56.04	21.89	:	LYS O 208	-23.58	-23.58	22.03
SER N 209	-25.75	-56.67	21.30	:	SER CA 209	-25.56	-25.56	20.74
SER CB 209	-26.86	-58.46	20.24	:	SER OG 209	-27.49	-27.49	21.51
SER C 209	-24.55	-57.92	19.65	:	SER O 209	-23.57	-23.57	19.72

15/32

III 1.15

SER N	210	-24.84	-56.91	18.81	:	SER CA	210	-24.14	-24.14	17.55
SER CB	210	-24.79	-55.56	16.74	:	SER OG	210	-26.24	-26.24	16.62
SER C	210	-22.69	-56.40	17.84	:	SER O	210	-21.85	-21.85	17.14
SER N	211	-22.43	-55.62	18.90	:	SER CA	211	-21.06	-21.06	19.26
SER CB	211	-21.18	-53.82	19.82	:	SER OG	211	-22.03	-22.03	19.04
SER C	211	-20.55	-56.28	20.30	:	SER O	211	-21.06	-21.06	20.27
ARG N	212	-19.64	-55.88	21.24	:	ARG CA	212	-19.04	-19.04	22.40
ARG CB	212	-19.73	-57.98	22.87	:	ARG CG	212	-21.16	-21.16	23.41
ARG CD	212	-21.77	-59.17	22.72	:	ARG NE	212	-23.25	-23.25	22.62
ARG CZ	212	-24.10	-59.38	23.70	:	ARG NH1	212	-25.47	-25.47	23.54
ARG NH2	212	-23.53	-59.40	24.98	:	ARG C	212	-17.62	-17.62	22.00
ARG OT1	212	-16.65	-56.67	22.70	:	ARG OT2	212	-17.56	-17.56	21.00
ASN CB	220	-3.63	-53.54	26.53	:	ASN CG	220	-4.61	-4.61	27.75
ASN OD1	220	-5.39	-52.66	28.00	:	ASN ND2	220	-4.60	-4.60	28.56
ASN C	220	-2.45	-51.28	26.97	:	ASN O	220	-1.34	-1.34	26.60
ASN N	220	-2.82	-52.06	24.65	:	ASN CA	220	-3.41	-3.41	25.99
THR N	221	-2.92	-51.16	28.19	:	THR CA	221	-2.36	-2.36	29.22
THR CB	221	-3.37	-50.58	30.35	:	THR OG1	221	-4.72	-4.72	29.83
THR CG2	221	-3.28	-49.38	31.32	:	THR C	221	-0.90	-0.90	29.67
THR O	221	-0.28	-51.48	29.55	:	ILE N	222	-0.28	-0.28	30.16
ILE CA	222	1.02	-49.41	30.76	:	ILE CB	222	2.12	2.12	29.77
ILE CG2	222	2.01	-47.64	29.26	:	ILE CG1	222	3.44	3.44	30.50
ILE CD1	222	4.70	-48.79	29.65	:	ILE C	222	0.98	0.98	31.85
ILE O	222	0.40	-47.29	31.64	:	GLY N	223	1.49	1.49	33.04
GLY CA	223	1.38	-47.40	34.00	:	GLY C	223	1.18	1.18	35.40
GLY O	223	0.89	-49.16	35.54	:	ASN N	224	1.23	1.23	36.42
ASN CA	224	1.45	-47.62	37.75	:	ASN CB	224	2.90	2.90	38.00
ASN CG	224	3.38	-45.94	38.17	:	ASN OD1	224	2.60	2.60	38.26
ASN ND2	224	4.71	-45.80	38.28	:	ASN C	224	0.57	0.57	38.76
ASN O	224	-0.55	-46.64	38.42	:	GLU N	225	1.00	1.00	39.97
GLU CA	225	0.17	-46.01	40.98	:	GLU CB	225	0.87	0.87	42.36
GLU CG	225	1.73	-47.04	42.87	:	GLU CD	225	3.18	3.18	42.26
GLU OE1	225	3.37	-47.69	41.13	:	GLU OE2	225	4.11	4.11	42.99
GLU C	225	-0.24	-44.56	40.63	:	GLU O	225	-1.27	-1.27	41.14
PHE N	226	0.53	-43.83	39.81	:	PHE CA	226	0.27	0.27	39.57
PHE CB	226	1.49	-41.64	39.60	:	PHE CG	226	2.30	2.30	40.80
PHE CD1	226	3.13	-42.94	40.85	:	PHE CD2	226	2.20	2.20	41.81
PHE CE1	226	3.90	-43.11	41.96	:	PHE CE2	226	2.97	2.97	42.92
PHE CZ	226	3.83	-42.21	42.99	:	PHE C	226	-0.38	-0.38	38.26
PHE O	226	-0.82	-40.89	38.08	:	GLY N	227	-0.27	-0.27	37.26
GLY CA	227	-0.95	-42.66	36.02	:	GLY C	227	-0.88	-0.88	35.17
GLY O	227	-0.09	-44.77	35.49	:	ASN N	228	-1.66	-1.66	34.14
ASN CA	228	-1.38	-45.14	33.23	:	ASN CB	228	-1.77	-1.77	33.78
ASN CG	228	-3.14	-46.74	34.35	:	ASN OD1	228	-4.14	-4.14	33.82
ASN ND2	228	-3.17	-47.51	35.44	:	ASN C	228	-2.10	-2.10	31.97
ASN O	228	-2.97	-43.95	31.93	:	LEU N	229	-1.38	-1.38	30.96
LEU CA	229	-1.54	-44.92	29.56	:	LEU CB	229	-0.13	-0.13	29.09
LEU CG	229	0.32	-43.99	27.78	:	LEU CD1	229	1.82	1.82	27.80
LEU CD2	229	-0.01	-44.89	26.65	:	LEU C	229	-2.10	-2.10	28.78
LEU O	229	-1.41	-47.11	28.73	:	THR N	230	-3.25	-3.25	28.11
THR CA	230	-3.60	-47.21	27.31	:	THR CB	230	-4.69	-4.69	28.12
THR OG1	230	-4.96	-49.13	27.32	:	THR CG2	230	-5.95	-5.95	28.42
THR C	230	-3.99	-46.79	25.88	:	THR O	230	-5.11	-5.11	25.53
GLU N	231	-2.86	-46.84	25.15	:	GLU CA	231	-2.62	-2.62	23.70
GLU CB	231	-1.12	-46.64	23.50	:	GLU CG	231	-0.49	-0.49	22.53
GLU CD	231	0.30	-44.52	23.16	:	GLU OE1	231	1.49	1.49	23.33
GLU OE2	231	-0.18	-43.40	23.45	:	GLU C	231	-3.21	-3.21	22.85
GLU O	231	-3.09	-48.90	23.28	:	ARG N	232	-3.78	-3.78	21.67
ARG CA	232	-4.30	-48.65	20.79	:	ARG CB	232	-5.79	-5.79	21.15

III - 1.16.

ARG CG 232	-6.85	-47.96	21.46	:	ARG CD 232	-8.00	-8.00	22.47
ARG NE 232	-8.92	-47.23	22.81	:	ARG CZ 232	-8.52	-8.52	23.58
ARG NH1 232	-9.35	-45.17	23.79	:	ARG NH2 232	-7.35	-7.35	24.27
ARG C 232	-4.25	-48.12	19.35	:	ARG O 232	-4.69	-4.69	19.19
THR N 233	-3.73	-48.78	18.28	:	THR CA 233	-3.62	-3.62	17.01
THR CB 233	-2.17	-48.08	16.41	:	THR OG1 233	-2.13	-2.13	15.30
THR CG2 233	-1.14	-48.51	17.43	:	THR C 233	-4.57	-4.57	15.98
THR O 233	-4.88	-49.78	16.03	:	ASP N 234	-4.97	-4.97	15.02
ASP CA 234	-5.81	-48.29	13.94	:	ASP CB 234	-6.97	-6.97	13.64
ASP CG 234	-7.66	-47.55	12.30	:	ASP OD1 234	-8.86	-8.86	12.27
ASP OD2 234	-7.07	-47.39	11.23	:	ASP C 234	-4.84	-4.84	12.80
ASP O 234	-4.30	-47.12	12.60	:	ASN N 235	-4.57	-4.57	11.96
ASN CA 235	-3.64	-48.91	10.92	:	ASN CB 235	-2.35	-2.35	10.86
ASN CG 235	-1.49	-49.33	9.62	:	ASN OD1 235	-1.82	-1.82	8.80
ASN ND2 235	-0.31	-49.97	9.47	:	ASN C 235	-4.43	-4.43	9.66
ASN O 235	-4.34	-50.11	8.98	:	SER N 236	-5.24	-5.24	9.39
SER CA 236	-6.03	-48.05	8.17	:	SER CB 236	-7.12	-7.12	8.20
SER OG 236	-8.00	-49.08	9.35	:	SER C 236	-6.64	-6.64	8.36
SER O 236	-7.88	-46.40	8.30	:	LEU N 237	-5.68	-5.68	8.74
LEU CA 237	-5.86	-44.50	9.29	:	LEU CB 237	-6.75	-6.75	10.48
LEU CG 237	-8.19	-44.14	10.16	:	LEU CD1 237	-8.96	-8.96	11.40
LEU CD2 237	-8.38	-42.70	9.69	:	LEU C 237	-4.47	-4.47	9.82
LEU O 237	-3.94	-43.17	9.64	:	ASN N 238	-3.86	-3.86	10.46
ASN CA 238	-2.50	-45.17	10.93	:	ASN CB 238	-1.67	-1.67	9.68
ASN CG 238	-0.31	-44.40	9.89	:	ASN OD1 238	0.29	0.29	9.03
ASN ND2 238	0.35	-44.56	11.03	:	ASN C 238	-2.52	-2.52	11.91
ASN O 238	-1.76	-43.01	11.87	:	VAL N 239	-3.45	-3.45	12.86
VAL CA 239	-3.76	-43.13	13.90	:	VAL CB 239	-5.19	-5.19	13.68
VAL CG1 239	-5.83	-41.98	14.85	:	VAL CG2 239	-5.14	-5.14	12.56
VAL C 239	-3.58	-43.91	15.20	:	VAL O 239	-3.80	-3.80	15.23
LEU N 240	-3.19	-43.34	16.32	:	LEU CA 240	-3.07	-3.07	17.60
LEU CB 240	-1.75	-43.57	18.07	:	LEU CG 240	-0.83	-0.83	19.08
LEU CD1 240	0.36	-44.71	18.37	:	LEU CD2 240	-0.27	-0.27	19.91
LEU C 240	-4.27	-43.54	18.44	:	LEU O 240	-4.50	-4.50	18.32
ILE N 241	-5.13	-44.19	19.24	:	ILE CA 241	-6.14	-6.14	20.02
ILE CB 241	-7.53	-44.12	19.92	:	ILE CG2 241	-8.50	-8.50	20.76
ILE CG1 241	-8.03	-44.07	18.52	:	ILE CD1 241	-9.07	-9.07	18.39
ILE C 241	-5.61	-43.75	21.41	:	ILE O 241	-5.86	-5.86	22.00
SER N 242	-4.84	-42.83	21.96	:	SER CA 242	-4.23	-4.23	23.26
SER CB 242	-2.89	-42.33	23.24	:	SER OG 242	-2.74	-2.74	23.89
SER C 242	-5.18	-42.50	24.33	:	SER O 242	-6.08	-6.08	24.03
SER N 243	-4.98	-42.78	25.60	:	SER CA 243	-5.95	-5.95	26.62
SER CB 243	-6.88	-43.62	26.47	:	SER OG 243	-7.79	-7.79	27.53
SER C 243	-5.10	-42.48	27.86	:	SER O 243	-4.61	-4.61	28.18
ILE N 244	-4.89	-41.37	28.56	:	ILE CA 244	-3.88	-3.88	29.62
ILE CB 244	-2.91	-40.11	29.23	:	ILE CG2 244	-1.98	-1.98	30.33
ILE CG1 244	-2.14	-40.57	28.08	:	ILE CD1 244	-1.32	-1.32	27.55
ILE C 244	-4.58	-40.84	30.91	:	ILE O 244	-5.32	-5.32	30.80
GLU N 245	-4.45	-41.43	32.09	:	GLU CA 245	-5.05	-5.05	33.27
GLU CB 245	-6.16	-41.71	33.72	:	GLU CG 245	-5.74	-5.74	33.88
GLU CD 245	-6.95	-44.08	34.13	:	GLU OE1 245	-6.88	-6.88	34.98
GLU OE2 245	-7.98	-43.78	33.45	:	GLU C 245	-3.96	-3.96	34.31
GLU O 245	-3.11	-41.63	34.40	:	MET N 246	-3.86	-3.86	35.02
MET CA 246	-2.83	-39.38	35.98	:	MET CB 246	-1.90	-1.90	35.55
MET CG 246	-0.94	-38.81	34.55	:	MET SD 246	-0.39	-0.39	33.59
MET CE 246	0.79	-36.91	34.78	:	MET C 246	-3.49	-3.49	37.20
MET O 246	-4.41	-38.01	36.96	:	GLU N 247	-3.19	-3.19	38.46
GLU CA 247	-3.96	-38.40	39.44	:	GLU CB 247	-4.65	-4.65	40.32
GLU CG 247	-4.18	-40.09	41.64	:	GLU CD 247	-2.68	-2.68	41.69

17/32

III 17.

GLU OE1	247	-2.11	-40.54	42.82	:	GLU OE2	247	-2.13	-2.13	40.57
GLU C	247	-2.96	-37.51	40.08	:	GLU O	247	-1.77	-1.77	39.82
GLU N	248	-3.51	-36.50	40.72	:	GLU CA	248	-2.82	-2.82	41.20
GLU CB	248	-3.65	-34.79	42.35	:	GLU CG	248	-3.07	-3.07	43.28
GLU CD	248	-4.14	-32.94	44.08	:	GLU OE1	248	-5.20	-5.20	44.51
GLU OE2	248	-3.88	-31.72	44.27	:	GLU C	248	-1.35	-1.35	41.57
GLU O	248	-0.97	-36.26	42.30	:	GLY N	249	-0.42	-0.42	41.09
GLY CA	249	0.96	-34.71	41.50	:	GLY C	249	1.77	1.77	40.56
GLY O	249	2.96	-35.28	40.42	:	ALA N	250	1.24	1.24	39.88
ALA CA	250	2.03	-37.48	39.00	:	ALA CB	250	1.18	1.18	38.34
ALA C	250	2.71	-36.73	37.89	:	ALA O	250	2.20	2.20	37.49
LEU N	251	3.81	-37.20	37.35	:	LEU CA	251	4.54	4.54	36.34
LEU CB	251	5.85	-36.07	36.91	:	LEU CG	251	6.99	6.99	36.05
LEU CD1	251	6.59	-34.20	35.53	:	LEU CD2	251	8.27	8.27	36.84
LEU C	251	4.74	-37.53	35.25	:	LEU O	251	5.11	5.11	35.57
PHE N	252	4.47	-37.25	33.99	:	PHE CA	252	4.76	4.76	32.91
PHE CB	252	3.79	-37.91	31.78	:	PHE CG	252	3.68	3.68	30.67
PHE CD1	252	4.70	-39.84	30.39	:	PHE CD2	252	2.50	2.50	29.97
PHE CE1	252	4.55	-40.79	29.40	:	PHE CE2	252	2.38	2.38	28.98
PHE CZ	252	3.40	-40.84	28.68	:	PHE C	252	6.14	6.14	32.60
PHE O	252	6.27	-36.50	32.10	:	VAL N	253	7.19	7.19	32.89
VAL CA	253	8.57	-37.94	32.78	:	VAL CB	253	9.53	9.53	33.26
VAL CG1	253	9.21	-39.42	34.70	:	VAL CG2	253	9.42	9.42	32.40
VAL C	253	8.95	-37.45	31.39	:	VAL O	253	8.31	8.31	30.43
PRO N	254	9.93	-36.54	31.20	:	PRO CD	254	10.71	10.71	32.26
PRO CA	254	10.42	-36.11	29.89	:	PRO CB	254	11.78	11.78	30.26
PRO CG	254	11.57	-34.89	31.58	:	PRO C	254	10.45	10.45	28.83
PRO O	254	11.05	-38.25	29.06	:	HIS N	255	9.80	9.80	27.69
HIS CA	255	9.87	-38.26	26.73	:	HIS CB	255	8.84	8.84	27.08
HIS CG	255	7.43	-38.77	27.09	:	HIS CD2	255	6.45	6.45	26.17
HIS ND1	255	6.93	-38.04	28.04	:	HIS CE1	255	5.69	5.69	27.74
HIS NE2	255	5.40	-38.35	26.62	:	HIS C	255	9.56	9.56	25.37
HIS O	255	9.27	-36.52	25.28	:	TYR N	256	9.55	9.55	24.32
TYR CA	256	9.08	-38.01	23.04	:	TYR CB	256	10.21	10.21	22.34
TYR CG	256	11.40	-38.11	21.88	:	TYR CD1	256	11.27	11.27	20.88
TYR CE1	256	12.33	-39.72	20.42	:	TYR CD2	256	12.61	12.61	22.44
TYR CE2	256	13.68	-38.57	21.99	:	TYR CZ	256	13.52	13.52	20.99
TYR OH	256	14.56	-40.24	20.59	:	TYR C	256	8.58	8.58	22.21
TYR O	256	8.97	-40.27	22.55	:	TYR N	257	7.79	7.79	21.15
TYR CA	257	7.34	-40.12	20.32	:	TYR CB	257	5.86	5.86	19.99
TYR CG	257	4.86	-40.41	21.02	:	TYR CD1	257	3.71	3.71	20.65
TYR CE1	257	2.86	-41.66	21.60	:	TYR CD2	257	5.14	5.14	22.36
TYR CE2	257	4.32	-40.86	23.32	:	TYR CZ	257	3.20	3.20	22.93
TYR OH	257	2.53	-42.22	23.92	:	TYR C	257	8.23	8.23	19.09
TYR O	257	8.48	-38.75	18.80	:	SER N	258	8.86	8.86	18.38
SER CA	258	9.60	-40.42	17.19	:	SER CB	258	10.56	10.56	16.90
SER OG	258	9.98	-42.77	16.94	:	SER C	258	8.61	8.61	16.09
SER O	258	7.73	-41.10	16.16	:	LYS N	259	8.51	8.51	15.05
LYS CA	259	7.40	-39.58	14.06	:	LYS CB	259	7.72	7.72	13.01
LYS CG	259	8.02	-42.13	13.44	:	LYS CD	259	7.88	7.88	12.29
LYS CE	259	6.51	-43.06	11.68	:	LYS NZ	259	5.57	5.57	12.77
LYS C	259	6.00	-39.89	14.53	:	LYS O	259	5.56	5.56	14.37
ALA N	260	5.27	-39.02	15.20	:	ALA CA	260	3.86	3.86	15.59
ALA CB	260	3.68	-40.36	16.65	:	ALA C	260	3.42	3.42	16.21
ALA O	260	3.93	-37.52	17.24	:	ILE N	261	2.55	2.55	15.53
ILE CA	261	2.17	-35.88	16.01	:	ILE CB	261	1.81	1.81	14.80
ILE CG2	261	1.32	-33.71	15.25	:	ILE CG1	261	2.99	2.99	13.92
ILE CD1	261	2.54	-34.49	12.57	:	ILE C	261	1.00	1.00	16.92
ILE O	261	0.04	-36.72	16.40	:	VAL N	262	1.05	1.05	18.22

18/32

III 1.10.

VAL CA	262	-0.01	-36.27	19.14	:	VAL CB	262	0.64	0.64	20.39
VAL CG1	262	-0.32	-36.96	21.50	:	VAL CG2	262	1.28	1.28	20.07
VAL C	262	-0.80	-35.03	19.38	:	VAL O	262	-0.20	-0.20	19.65
ILE N	263	-2.10	-35.06	19.21	:	ILE CA	263	-2.99	-2.99	19.50
ILE CB	263	-4.14	-33.89	18.46	:	ILE CG2	263	-5.06	-5.06	18.81
ILE CG1	263	-3.62	-33.72	17.05	:	ILE CD1	263	-4.65	-4.65	15.97
ILE C	263	-3.52	-34.41	20.86	:	ILE O	263	-4.12	-4.12	20.88
LEU N	264	-3.26	-33.74	22.00	:	LEU CA	264	-3.71	-3.71	23.32
LEU CB	264	-2.75	-33.85	24.43	:	LEU CG	264	-1.82	-1.82	25.11
LEU CD1	264	-1.72	-34.21	26.49	:	LEU CD2	264	-2.30	-2.30	25.23
LEU C	264	-4.87	-33.28	23.67	:	LEU O	264	-4.68	-4.68	23.58
VAL N	265	-6.02	-33.78	24.07	:	VAL CA	265	-7.12	-7.12	24.48
VAL CB	265	-8.35	-33.09	23.50	:	VAL CG1	265	-8.33	-8.33	22.79
VAL CG2	265	-9.66	-32.99	24.23	:	VAL C	265	-7.40	-7.40	25.90
VAL O	265	-7.44	-34.57	26.21	:	VAL N	266	-7.52	-7.52	26.81
VAL CA	266	-7.68	-32.81	28.19	:	VAL CB	266	-6.89	-6.89	29.18
VAL CG1	266	-6.24	-30.77	28.44	:	VAL CG2	266	-7.75	-7.75	30.22
VAL C	266	-9.18	-32.85	28.40	:	VAL O	266	-9.93	-9.93	27.81
ASN N	267	-9.63	-33.82	29.17	:	ASN CA	267	-11.03	-11.03	29.32
ASN CB	267	-11.28	-35.55	29.20	:	ASN CG	267	-11.24	-11.24	27.78
ASN OD1	267	-11.63	-35.27	26.90	:	ASN ND2	267	-10.83	-10.83	27.45
ASN C	267	-11.79	-33.61	30.54	:	ASN O	267	-12.95	-12.95	30.37
GLU N	268	-11.17	-33.91	31.69	:	GLU CA	268	-11.61	-11.61	33.09
GLU CB	268	-12.21	-35.12	33.67	:	GLU CG	268	-12.50	-12.50	35.19
GLU CD	268	-11.48	-36.55	36.05	:	GLU OE1	268	-10.45	-10.45	36.58
GLU OE2	268	-11.73	-37.79	36.22	:	GLU C	268	-10.24	-10.24	33.68
GLU O	268	-9.30	-34.20	33.40	:	GLY N	269	-10.03	-10.03	34.31
GLY CA	269	-8.82	-32.06	35.10	:	GLY C	269	-7.95	-7.95	34.72
GLY O	269	-8.19	-30.31	33.69	:	GLU N	270	-6.95	-6.95	35.51
GLU CA	270	-5.97	-29.54	35.18	:	GLU CB	270	-5.85	-5.85	36.21
GLU CG	270	-6.99	-27.51	36.38	:	GLU CD	270	-8.27	-8.27	36.78
GLU OE1	270	-8.33	-28.86	37.85	:	GLU OE2	270	-9.21	-9.21	35.97
GLU C	270	-4.56	-30.12	35.05	:	GLU O	270	-4.22	-4.22	35.74
ALA N	271	-3.61	-29.65	34.25	:	ALA CA	271	-2.29	-2.29	34.19
ALA CB	271	-2.18	-31.38	33.19	:	ALA C	271	-1.33	-1.33	33.72
ALA O	271	-1.76	-28.26	33.11	:	HIS N	272	-0.03	-0.03	33.90
HIS CA	272	0.89	-28.27	33.49	:	HIS CB	272	1.63	1.63	34.72
HIS CG	272	2.91	-27.25	34.41	:	HIS CD2	272	3.11	3.11	34.59
HIS ND1	272	4.00	-27.75	33.88	:	HIS CE1	272	4.84	4.84	33.72
HIS NE2	272	4.29	-25.68	34.16	:	HIS C	272	1.72	1.72	32.44
HIS O	272	2.20	-30.06	32.76	:	VAL N	273	2.03	2.03	31.24
VAL CA	273	2.79	-29.24	30.27	:	VAL CB	273	1.88	1.88	29.05
VAL CG1	273	1.40	-28.30	28.43	:	VAL CG2	273	2.64	2.64	28.01
VAL C	273	4.01	-28.44	29.88	:	VAL O	273	3.99	3.99	30.12
GLU N	274	5.13	-29.03	29.46	:	GLU CA	274	6.27	6.27	29.00
GLU CB	274	7.44	-28.24	29.97	:	GLU CG	274	7.10	7.10	31.43
GLU CD	274	8.08	-27.57	32.31	:	GLU OE1	274	7.64	7.64	33.08
GLU OE2	274	9.30	-27.79	32.23	:	GLU C	274	6.77	6.77	27.79
GLU O	274	7.00	-30.21	27.91	:	LEU N	275	6.91	6.91	26.63
LEU CA	275	7.31	-28.97	25.36	:	LEU CB	275	6.29	6.29	24.33
LEU CG	275	5.93	-29.14	23.02	:	LEU CD1	275	6.27	6.27	21.89
LEU CD2	275	6.65	-30.43	22.88	:	LEU C	275	8.66	8.66	25.11
LEU O	275	8.77	-27.19	25.43	:	VAL N	276	9.70	9.70	24.59
VAL CA	276	10.96	-28.38	24.29	:	VAL CB	276	12.15	12.15	24.89
VAL CG1	276	13.50	-28.55	24.44	:	VAL CG2	276	12.07	12.07	26.39
VAL C	276	11.13	-28.34	22.80	:	VAL O	276	11.17	11.17	22.09
GLY N	277	11.26	-27.16	22.28	:	GLY CA	277	11.22	11.22	20.83
GLY C	277	12.42	-26.27	20.32	:	GLY O	277	13.19	13.19	21.14
PRO N	278	12.68	-26.17	19.03	:	PRO CD	278	11.91	11.91	18.00

19/32

III 1.19

PRO CA	278	13.80	-25.39	18.52	:	PRO CB	278	14.14	14.14	17.23
PRO CG	278	12.73	-26.38	16.77	:	PRO C	278	13.26	13.26	18.44
PRO O	278	12.09	-23.75	18.13	:	LYS N	279	14.11	14.11	18.72
LYS CA	279	13.66	-21.64	18.99	:	LYS CB	279	14.85	14.85	19.60
LYS CG	279	14.66	-19.49	19.77	:	LYS CD	279	16.02	16.02	19.78
LYS CE	279	16.41	-18.44	21.24	:	LYS NZ	279	17.10	17.10	21.89
LYS C	279	13.20	-21.04	17.69	:	LYS O	279	13.98	13.98	16.75
GLY N	280	11.90	-20.86	17.59	:	GLY CA	280	11.24	11.24	16.37
GLY C	280	11.56	-21.30	15.08	:	GLY O	280	10.83	10.83	14.18
ASN N	281	12.45	-22.36	14.82	:	ASN CA	281	12.77	12.77	13.45
ASN CB	281	12.81	-21.85	12.40	:	ASN CG	281	14.20	14.20	12.42
ASN OD1	281	14.83	-21.15	11.34	:	ASN ND2	281	14.72	14.72	13.59
ASN C	281	14.12	-23.72	13.19	:	ASN O	281	15.01	15.01	14.01
LYS N	282	14.30	-24.10	11.91	:	LYS CA	282	15.44	15.44	11.26
LYS CB	282	15.23	-25.00	9.67	:	LYS CG	282	16.16	16.16	8.76
LYS CD	282	17.00	-24.72	8.02	:	LYS CE	282	18.57	18.57	8.21
LYS NZ	282	19.33	-23.53	7.97	:	LYS C	282	16.70	16.70	11.48
LYS O	282	16.64	-22.86	11.65	:	GLU N	283	17.86	17.86	11.42
GLU CA	283	19.14	-24.13	11.85	:	GLU CB	283	19.57	19.57	11.17
GLU CG	283	21.12	-22.73	10.94	:	GLU CD	283	22.08	22.08	11.97
GLU OE1	283	22.70	-20.97	11.49	:	GLU OE2	283	22.25	22.25	13.19
GLU C	283	18.86	-23.83	13.33	:	GLU O	283	17.81	17.81	13.82
THR N	284	19.65	-23.13	14.13	:	THR CA	284	19.43	19.43	15.55
THR CB	284	18.09	-22.43	15.86	:	THR OG1	284	18.62	18.62	16.54
THR CG2	284	16.99	-23.14	16.65	:	THR C	284	19.47	19.47	16.10
THR O	284	18.84	-25.55	15.77	:	LEU N	285	20.51	20.51	16.90
LEU CA	285	20.65	-25.71	17.81	:	LEU CB	285	22.14	22.14	17.86
LEU CG	285	22.68	-27.39	17.30	:	LEU CD1	285	22.18	22.18	15.97
LEU CD2	285	24.13	-27.12	17.10	:	LEU C	285	20.13	20.13	19.10
LEU O	285	20.42	-25.57	20.19	:	GLU N	286	19.44	19.44	19.07
GLU CA	286	18.88	-23.32	20.26	:	GLU CB	286	18.70	18.70	20.15
GLU CG	286	19.99	-21.12	20.00	:	GLU CD	286	19.72	19.72	20.39
GLU OE1	286	19.72	-19.45	21.61	:	GLU OE2	286	19.34	19.34	19.54
GLU C	286	17.49	-23.85	20.58	:	GLU O	286	16.60	16.60	19.79
TYR N	287	17.27	-24.58	21.68	:	TYR CA	287	15.94	15.94	22.10
TYR CB	287	16.08	-26.36	22.91	:	TYR CG	287	16.93	16.93	22.16
TYR CD1	287	18.18	-27.70	22.64	:	TYR CE1	287	19.06	19.06	21.90
TYR CD2	287	16.51	-27.79	20.94	:	TYR CE2	287	17.36	17.36	20.18
TYR CZ	287	18.64	-28.84	20.64	:	TYR OH	287	19.55	19.55	19.74
TYR C	287	15.31	-23.94	22.94	:	TYR O	287	15.99	15.99	23.19
GLU N	288	14.03	-23.98	23.26	:	GLU CA	288	13.35	13.35	23.99
GLU CB	288	13.12	-21.89	22.99	:	GLU CG	288	12.36	12.36	23.42
GLU CD	288	11.21	-20.47	22.42	:	GLU OE1	288	10.21	10.21	22.64
GLU OE2	288	11.35	-19.69	21.43	:	GLU C	288	12.09	12.09	24.50
GLU O	288	11.59	-24.35	23.70	:	SER N	289	11.54	11.54	25.70
SER CA	289	10.34	-24.20	25.99	:	SER CB	289	10.39	10.39	27.30
SER OG	289	10.80	-24.25	28.45	:	SER C	289	9.05	9.05	26.02
SER O	289	8.98	-22.35	26.51	:	TYR N	290	8.02	8.02	25.56
TYR CA	290	6.65	-23.72	25.39	:	TYR CB	290	6.13	6.13	24.04
TYR CG	290	7.03	-23.76	22.91	:	TYR CD1	290	6.71	6.71	22.20
TYR CE1	290	7.52	-22.22	21.17	:	TYR CD2	290	8.15	8.15	22.57
TYR CE2	290	8.96	-24.07	21.55	:	TYR CZ	290	8.64	8.64	20.87
TYR OH	290	9.50	-22.46	19.92	:	TYR C	290	5.91	5.91	26.55
TYR O	290	5.68	-25.60	26.56	:	ARG N	291	5.68	5.68	27.65
ARG CA	291	5.03	-24.32	28.76	:	ARG CB	291	5.68	5.68	30.03
ARG CG	291	7.20	-23.95	30.12	:	ARG CD	291	7.60	7.60	31.54
ARG NE	291	9.03	-23.39	31.87	:	ARG CZ	291	10.04	10.04	31.53
ARG NH1	291	11.30	-23.90	31.88	:	ARG NH2	291	9.85	9.85	30.84
ARG C	291	3.60	-23.85	28.61	:	ARG O	291	3.39	3.39	27.95

20/32

III 1.20

ALA N	292	2.59	-24.46	29.19	:	ALA CA	292	1.24	1.24	29.05
ALA CB	292	0.67	-24.41	27.71	:	ALA C	292	0.47	0.47	30.16
ALA O	292	0.88	-25.75	30.61	:	GLU N	293	-0.68	-0.68	30.56
GLU CA	293	-1.37	-24.66	31.72	:	GLU CB	293	-1.55	-1.55	32.63
GLU CG	293	-1.15	-23.76	34.03	:	GLU CD	293	0.33	0.33	34.25
GLU OE1	293	1.24	-23.67	33.53	:	GLU OE2	293	0.58	0.58	35.22
GLU C	293	-2.69	-25.20	31.25	:	GLU O	293	-3.59	-3.59	31.06
LEU N	294	-2.84	-26.51	31.07	:	LEU CA	294	-4.00	-4.00	30.43
LEU CB	294	-3.60	-28.50	29.90	:	LEU CG	294	-2.38	-2.38	29.09
LEU CD1	294	-2.27	-29.95	28.48	:	LEU CD2	294	-2.48	-2.48	27.98
LEU C	294	-5.21	-27.35	31.32	:	LEU O	294	-5.01	-5.01	32.50
SER N	295	-6.45	-27.24	30.87	:	SER CA	295	-7.63	-7.63	31.67
SER CB	295	-7.96	-26.24	32.42	:	SER OG	295	-7.99	-7.99	31.58
SER C	295	-8.81	-27.99	30.83	:	SER O	295	-8.76	-8.76	29.61
LYS N	296	-9.95	-28.41	31.35	:	LYS CA	296	-11.03	-11.03	30.63
LYS CB	296	-12.41	-28.73	31.14	:	LYS CG	296	-13.22	-13.22	31.39
LYS CD	296	-14.71	-29.79	31.59	:	LYS CE	296	-15.43	-15.43	30.32
LYS NZ	296	-14.55	-29.69	29.16	:	LYS C	296	-11.26	-11.26	29.17
LYS O	296	-11.99	-29.98	28.86	:	ASP N	297	-10.97	-10.97	28.22
ASP CA	297	-11.14	-28.58	26.81	:	ASP CB	297	-12.38	-12.38	26.27
ASP CG	297	-13.48	-29.07	26.25	:	ASP OD1	297	-14.59	-14.59	26.57
ASP OD2	297	-13.29	-30.26	25.97	:	ASP C	297	-10.03	-10.03	25.95
ASP O	297	-10.20	-27.58	24.81	:	ASP N	298	-8.87	-8.87	26.55
ASP CA	298	-7.72	-27.36	25.91	:	ASP CB	298	-6.72	-6.72	26.93
ASP CG	298	-6.97	-25.69	27.70	:	ASP OD1	298	-6.35	-6.35	28.71
ASP OD2	298	-7.78	-24.88	27.33	:	ASP C	298	-7.11	-7.11	25.05
ASP O	298	-7.13	-29.58	25.43	:	VAL N	299	-6.50	-6.50	23.93
VAL CA	299	-5.80	-29.17	23.26	:	VAL CB	299	-6.45	-6.45	21.85
VAL CG1	299	-7.82	-29.01	21.71	:	VAL CG2	299	-5.55	-5.55	20.72
VAL C	299	-4.41	-28.63	23.13	:	VAL O	299	-4.21	-4.21	22.92
PHE N	300	-3.41	-29.44	23.33	:	PHE CA	300	-2.03	-2.03	23.18
PHE CB	300	-1.28	-29.24	24.50	:	PHE CG	300	0.12	0.12	24.53
PHE CD1	300	0.35	-27.31	24.88	:	PHE CD2	300	1.21	1.21	24.23
PHE CE1	300	1.62	-26.80	24.93	:	PHE CE2	300	2.47	2.47	24.28
PHE CZ	300	2.69	-27.57	24.63	:	PHE C	300	-1.52	-1.52	22.12
PHE O	300	-1.88	-31.17	22.32	:	VAL N	301	-0.80	-0.80	21.03
VAL CA	301	-0.27	-30.61	20.06	:	VAL CB	301	-0.58	-0.58	18.58
VAL CG1	301	-0.81	-28.75	18.48	:	VAL CG2	301	0.56	0.56	17.63
VAL C	301	1.22	-30.66	20.34	:	VAL O	301	1.86	1.86	20.56
ILE N	302	1.78	-31.85	20.41	:	ILE CA	302	3.16	3.16	20.76
ILE CB	302	3.16	-33.28	21.83	:	ILE CG2	302	4.57	4.57	22.25
ILE CG1	302	2.38	-32.90	23.07	:	ILE CD1	302	1.85	1.85	23.87
ILE C	302	3.72	-32.58	19.41	:	ILE O	302	3.25	3.25	18.95
PRO N	303	4.58	-31.85	18.68	:	PRO CD	303	5.09	5.09	19.04
PRO CA	303	5.10	-32.20	17.36	:	PRO CB	303	5.91	5.91	16.97
PRO CG	303	5.32	-29.90	17.71	:	PRO C	303	5.88	5.88	17.37
PRO O	303	5.68	-34.23	18.33	:	ALA N	304	6.81	6.81	16.46
ALA CA	304	7.25	-35.21	16.55	:	ALA CB	304	6.95	6.95	15.21
ALA C	304	8.60	-35.63	17.01	:	ALA O	304	8.85	8.85	16.82
ALA N	305	9.64	-34.97	17.44	:	ALA CA	305	10.64	10.64	18.28
ALA CB	305	12.02	-35.52	17.84	:	ALA C	305	10.35	10.35	19.42
ALA O	305	9.23	-34.88	19.91	:	TYR N	306	11.08	11.08	19.97
TYR CA	306	10.44	-32.79	20.87	:	TYR CB	306	9.17	9.17	20.31
TYR CG	306	9.27	-31.02	19.19	:	TYR CD1	306	9.69	9.69	17.93
TYR CE1	306	9.72	-30.55	16.86	:	TYR CD2	306	8.86	8.86	19.41
TYR CE2	306	8.89	-28.88	18.34	:	TYR CZ	306	9.31	9.31	17.09
TYR OH	306	9.30	-28.45	15.98	:	TYR C	306	9.97	9.97	22.20
TYR O	306	8.89	-33.85	22.35	:	PRO N	307	10.80	10.80	23.19
PRO CD	307	12.15	-32.69	23.06	:	PRO CA	307	10.54	10.54	24.52

21/32

III. 1.21.

PRO CB	307	11.80	-33.33	25.21	:	PRO CG	307	12.77	12.77	24.08
PRO C	307	9.32	-33.05	25.17	:	PRO O	307	9.21	9.21	25.13
VAL N	308	8.39	-33.77	25.75	:	VAL CA	308	7.27	7.27	26.42
VAL CB	308	6.01	-33.42	25.57	:	VAL CG1	308	5.74	5.74	25.61
VAL CG2	308	4.79	-32.68	26.06	:	VAL C	308	7.25	7.25	27.82
VAL O	308	7.74	-34.81	28.01	:	ALA N	309	6.75	6.75	28.87
ALA CA	309	6.69	-33.65	30.23	:	ALA CB	309	7.77	7.77	31.14
ALA C	309	5.39	-33.11	30.74	:	ALA O	309	5.20	5.20	30.59
ILE N	310	4.46	-33.89	31.25	:	ILE CA	310	3.13	3.13	31.58
ILE CB	310	2.07	-34.28	30.92	:	ILE CG2	310	0.69	0.69	31.29
ILE CG1	310	2.15	-34.13	29.44	:	ILE CD1	310	1.19	1.19	28.63
ILE C	310	3.03	-33.51	33.08	:	ILE O	310	3.40	3.40	33.58
LYS N	311	2.66	-32.55	33.90	:	LYS CA	311	2.46	2.46	35.32
LYS CB	311	3.29	-31.81	36.09	:	LYS CG	311	2.97	2.97	37.54
LYS CD	311	4.15	-31.35	38.33	:	LYS CE	311	3.63	3.63	39.75
LYS NZ	311	2.99	-32.32	40.26	:	LYS C	311	1.00	1.00	35.69
LYS O	311	0.39	-31.60	35.38	:	ALA N	312	0.38	0.38	36.35
ALA CA	312	-1.00	-33.42	36.74	:	ALA CB	312	-1.58	-1.58	37.09
ALA C	312	-1.10	-32.53	37.95	:	ALA O	312	-0.30	-0.30	38.88
THR N	313	-2.06	-31.65	37.94	:	THR CA	313	-2.25	-2.25	38.93
THR CB	313	-2.45	-29.36	38.12	:	THR OG1	313	-1.14	-1.14	38.02
THR CG2	313	-3.30	-28.26	38.69	:	THR C	313	-3.43	-3.43	39.79
THR O	313	-3.54	-30.58	40.93	:	SER N	314	-4.38	-4.38	39.17
SER CA	314	-5.50	-32.33	39.78	:	SER CB	314	-6.65	-6.65	39.50
SER OG	314	-6.57	-30.97	38.19	:	SER C	314	-5.57	-5.57	39.08
SER O	314	-4.72	-33.96	38.25	:	ASN N	315	-6.49	-6.49	39.33
ASN CA	315	-6.57	-35.81	38.58	:	ASN CB	315	-7.58	-7.58	39.17
ASN CG	315	-7.24	-37.18	40.58	:	ASN OD1	315	-6.32	-6.32	41.20
ASN ND2	315	-7.91	-38.13	41.20	:	ASN C	315	-7.07	-7.07	37.24
ASN O	315	-7.97	-34.52	37.22	:	VAL N	316	-6.47	-6.47	36.18
VAL CA	316	-6.80	-35.46	34.86	:	VAL CB	316	-5.62	-5.62	34.63
VAL CG1	316	-4.31	-35.18	34.63	:	VAL CG2	316	-5.89	-5.89	33.38
VAL C	316	-7.01	-36.58	33.85	:	VAL O	316	-6.33	-6.33	33.93
ASN N	317	-7.91	-36.52	32.89	:	ASN CA	317	-8.00	-8.00	31.92
ASN CB	317	-9.37	-38.10	31.75	:	ASN CG	317	-9.95	-9.95	33.07
ASN OD1	317	-9.26	-39.33	33.77	:	ASN ND2	317	-11.21	-11.21	33.48
ASN C	317	-7.64	-37.02	30.59	:	ASN O	317	-8.31	-8.31	30.27
PHE N	318	-6.70	-37.49	29.78	:	PHE CA	318	-6.47	-6.47	28.48
PHE CB	318	-4.98	-36.68	28.31	:	PHE CG	318	-4.26	-4.26	29.28
PHE CD1	318	-3.62	-36.26	30.38	:	PHE CD2	318	-4.21	-4.21	29.06
PHE CE1	318	-2.92	-35.45	31.24	:	PHE CE2	318	-3.51	-3.51	29.92
PHE CZ	318	-2.86	-34.11	31.02	:	PHE C	318	-6.99	-6.99	27.42
PHE O	318	-7.07	-39.09	27.75	:	THR N	319	-7.43	-7.43	26.20
THR CA	319	-7.67	-38.51	25.11	:	THR CB	319	-9.01	-9.01	24.39
THR OG1	319	-10.05	-38.69	25.25	:	THR CG2	319	-9.11	-9.11	23.17
THR C	319	-6.57	-38.07	24.14	:	THR O	319	-6.54	-6.54	23.90
GLY N	320	-5.65	-38.85	23.60	:	GLY CA	320	-4.68	-4.68	22.68
GLY C	320	-4.95	-38.90	21.33	:	GLY O	320	-5.44	-5.44	21.33
PHE N	321	-4.78	-38.28	20.16	:	PHE GA	321	-4.89	-4.89	18.89
PHE CB	321	-5.82	-38.32	17.89	:	PHE CG	321	-7.25	-7.25	18.34
PHE CD1	321	-7.95	-39.55	18.24	:	PHE CD2	321	-7.86	-7.86	18.90
PHE CE1	321	-9.23	-39.65	18.68	:	PHE CE2	321	-9.14	-9.14	19.35
PHE CZ	321	-9.82	-38.56	19.25	:	PHE C	321	-3.49	-3.49	18.34
PHE O	321	-2.99	-37.74	18.37	:	GLY N	322	-2.73	-2.73	17.90
GLY CA	322	-1.38	-39.59	17.41	:	GLY C	322	-1.47	-1.47	15.93
GLY O	322	-1.76	-40.92	15.49	:	ILE N	323	-1.34	-1.34	15.10
ILE CA	323	-1.45	-38.99	13.66	:	ILE CB	323	-1.89	-1.89	12.89
ILE CG2	323	-3.00	-36.95	13.62	:	ILE CG1	323	-0.74	-0.74	12.73
ILE CD1	323	-0.26	-36.78	11.28	:	ILE C	323	-0.06	-0.06	13.27

22/32

III 1.22

ILE O	323	0.91	-39.08	13.95	:	ASN N	324	0.08	0.08	12.18
ASN CA	324	1.36	-40.63	11.66	:	ASN CB	324	2.32	2.32	11.49
ASN CG	324	3.61	-39.91	10.86	:	ASN OD1	324	4.72	4.72	11.41
ASN ND2	324	3.45	-40.56	9.72	:	ASN C	324	1.97	1.97	12.57
ASN O	324	3.16	-41.93	12.70	:	ALA N	325	1.19	1.19	13.06
ALA CA	325	1.65	-43.50	14.07	:	ALA CB	325	0.47	0.47	14.92
ALA C	325	2.38	-44.76	13.70	:	ALA O	325	2.94	2.94	14.62
ASN N	326	2.55	-45.29	12.47	:	ASN CA	326	3.12	3.12	12.32
ASN CB	326	2.82	-47.23	10.93	:	ASN CG	326	1.29	1.29	10.67
ASN OD1	326	0.87	-47.01	9.56	:	ASN ND2	326	0.34	0.34	11.60
ASN C	326	4.61	-46.70	12.58	:	ASN O	326	5.38	5.38	12.23
ASN N	327	4.98	-47.71	13.34	:	ASN CA	327	6.33	6.33	13.83
ASN CB	327	7.35	-47.99	12.71	:	ASN CG	327	6.95	6.95	11.65
ASN OD1	327	6.82	-50.20	11.92	:	ASN ND2	327	6.69	6.69	10.43
ASN C	327	6.72	-46.68	14.64	:	ASN O	327	7.84	7.84	14.55
ASN N	328	5.77	-46.08	15.35	:	ASN CA	328	6.10	6.10	16.19
ASN CB	328	4.82	-44.35	16.70	:	ASN CG	328	5.09	5.09	17.74
ASN OD1	328	5.90	-42.44	17.53	:	ASN ND2	328	4.55	4.55	18.93
ASN C	328	6.97	-45.47	17.33	:	ASN O	328	6.94	6.94	17.50
ASN N	329	7.67	-44.78	18.22	:	ASN CA	329	8.52	8.52	19.22
ASN CB	329	9.89	-45.51	18.73	:	ASN CG	329	10.32	10.32	18.55
ASN OD1	329	9.58	-47.73	18.07	:	ASN ND2	329	11.54	11.54	18.93
ASN C	329	8.55	-44.47	20.37	:	ASN O	329	9.04	9.04	20.21
ARG N	330	8.14	-44.86	21.55	:	ARG CA	330	7.98	7.98	22.62
ARG CB	330	6.89	-44.41	23.51	:	ARG CG	330	6.19	6.19	24.26
ARG CD	330	5.11	-43.97	25.14	:	ARG NE	330	4.07	4.07	24.44
ARG CZ	330	3.99	-46.12	24.50	:	ARG NH1	330	2.99	2.99	23.89
ARG NH2	330	4.91	-46.84	25.15	:	ARG C	330	9.31	9.31	23.32
ARG O	330	9.70	-44.80	23.86	:	ASN N	331	10.09	10.09	23.31
ASN CA	331	11.41	-42.77	23.94	:	ASN CB	331	12.37	12.37	23.12
ASN CG	331	12.74	-42.83	21.95	:	ASN OD1	331	13.78	13.78	22.03
ASN ND2	331	12.06	-43.07	20.83	:	ASN C	331	11.38	11.38	25.30
ASN O	331	11.03	-40.96	25.28	:	LEU N	332	11.64	11.64	26.46
LEU CA	332	11.57	-42.06	27.71	:	LEU CB	332	10.95	10.95	28.72
LEU CG	332	9.51	-42.60	28.75	:	LEU CD1	332	8.74	8.74	27.67
LEU CD2	332	9.00	-43.07	30.05	:	LEU C	332	12.92	12.92	28.17
LEU O	332	13.92	-42.19	27.84	:	LEU N	333	13.02	13.02	28.84
LEU CA	333	14.30	-39.89	29.27	:	LEU CB	333	14.40	14.40	28.84
LEU CG	333	14.11	-38.13	27.39	:	LEU CD1	333	13.99	13.99	27.22
LEU CD2	333	15.19	-38.68	26.51	:	LEU C	333	14.51	14.51	30.78
LEU O	333	15.45	-39.45	31.34	:	ALA N	334	13.69	13.69	31.52
ALA CA	334	13.88	-40.85	32.93	:	ALA CB	334	13.17	13.17	33.65
ALA C	334	13.23	-42.15	33.31	:	ALA O	334	12.23	12.23	32.69
GLY N	335	13.75	-42.88	34.28	:	GLY CA	335	13.00	13.00	34.72
GLY C	335	13.54	-45.31	34.12	:	GLY O	335	14.56	14.56	33.42
LYS N	336	12.87	-46.42	34.49	:	LYS CA	336	13.33	13.33	34.04
LYS CB	336	13.04	-48.81	35.07	:	LYS CG	336	13.77	13.77	36.37
LYS CD	336	14.36	-49.56	37.16	:	LYS CE	336	13.32	13.32	37.51
LYS NZ	336	12.17	-50.26	38.34	:	LYS C	336	12.77	12.77	32.74
LYS O	336	13.56	-48.46	31.84	:	THR N	337	11.48	11.48	32.50
THR CA	337	11.01	-48.80	31.20	:	THR CB	337	9.55	9.55	31.29
THR OG1	337	9.28	-49.63	32.49	:	THR CG2	337	8.99	8.99	30.05
THR C	337	11.36	-47.82	30.07	:	THR O	337	11.31	11.31	30.29
ASP N	338	11.73	-48.28	28.88	:	ASP CA	338	12.03	12.03	27.76
ASP CB	338	10.67	-47.02	27.23	:	ASP CG	338	9.84	9.84	26.67
ASP OD1	338	8.62	-48.00	26.63	:	ASP OD2	338	10.42	10.42	26.30
ASP C	338	12.94	-46.16	27.89	:	ASP O	338	12.78	12.78	27.20
ASN N	339	13.99	-46.17	28.68	:	ASN CA	339	14.78	14.78	28.96
ASN CB	339	15.41	-45.12	30.33	:	ASN CG	339	16.10	16.10	30.71

23/32

III. 1.23.

ASN OD1	339	15.74	-43.20	31.69	:	ASN ND2	339	17.11	17.11	30.07
ASN C	339	15.87	-44.71	27.95	:	ASN O	339	17.00	17.00	28.27
VAL N	340	15.79	-43.98	26.82	:	VAL CA	340	16.89	16.89	25.85
VAL CB	340	16.79	-42.96	24.73	:	VAL CG1	340	16.23	16.23	23.70
VAL CG2	340	16.07	-41.69	24.99	:	VAL C	340	18.25	18.25	26.34
VAL O	340	19.19	-44.21	25.82	:	ILE N	341	18.36	18.36	27.36
ILE CA	341	19.68	-42.41	27.83	:	ILE CB	341	19.62	19.62	28.93
ILE CG2	341	21.04	-40.91	29.38	:	ILE CG1	341	19.00	19.00	28.36
ILE CD1	341	19.09	-38.77	29.21	:	ILE C	341	20.36	20.36	28.36
ILE O	341	21.45	-43.92	27.87	:	SER N	342	19.85	19.85	29.19
SER CA	342	20.74	-45.65	29.60	:	SER CB	342	20.18	20.18	30.79
SER OG	342	18.89	-46.79	30.44	:	SER C	342	20.95	20.95	28.51
SER O	342	21.92	-47.44	28.58	:	SER N	343	20.06	20.06	27.53
SER CA	343	20.31	-47.63	26.38	:	SER CB	343	19.10	19.10	25.46
SER OG	343	19.17	-48.62	24.43	:	SER C	343	21.53	21.53	25.63
SER O	343	22.27	-47.90	25.03	:	ILE N	344	21.78	21.78	25.64
ILE CA	344	22.97	-45.26	24.98	:	ILE CB	344	23.05	23.05	25.01
ILE CG2	344	24.45	-43.29	24.58	:	ILE CG1	344	22.02	22.02	24.09
ILE CD1	344	22.18	-41.61	23.95	:	ILE C	344	24.10	24.10	25.81
ILE O	344	25.02	-46.47	25.25	:	GLY N	345	24.01	24.01	27.15
GLY CA	345	25.05	-46.27	28.05	:	GLY C	345	24.85	24.85	28.29
GLY O	345	24.69	-48.28	29.40	:	ARG N	346	24.78	24.78	27.19
ARG CA	346	24.63	-49.89	27.12	:	ARG CB	346	23.20	23.20	27.33
ARG CG	346	23.31	-51.42	28.30	:	ARG CD	346	23.10	23.10	29.73
ARG NE	346	21.76	-50.34	29.79	:	ARG CZ	346	20.70	20.70	29.57
ARG NH1	346	19.46	-50.59	29.43	:	ARG NH2	346	20.88	20.88	29.57
ARG C	346	25.03	-50.26	25.70	:	ARG O	346	24.97	24.97	25.29
ALA N	347	25.29	-49.27	24.85	:	ALA CA	347	25.91	25.91	23.60
ALA CB	347	25.83	-48.29	22.79	:	ALA C	347	27.35	27.35	23.85
ALA O	347	27.92	-49.86	24.93	:	LEU N	348	27.98	27.98	22.82
LEU CA	348	29.23	-51.23	22.93	:	LEU CB	348	29.42	29.42	21.68
LEU CG	348	30.55	-53.03	21.63	:	LEU CD1	348	29.84	29.84	20.99
LEU CD2	348	31.83	-52.63	20.87	:	LEU C	348	30.24	30.24	23.02
LEU O	348	31.01	-50.06	22.08	:	ASP N	349	30.32	30.32	24.09
ASP CA	349	31.11	-48.12	24.11	:	ASP CB	349	31.23	31.23	22.75
ASP CG	349	30.00	-47.24	21.79	:	ASP OD1	349	28.86	28.86	22.25
ASP OD2	349	30.17	-47.02	20.58	:	ASP C	349	30.37	30.37	25.02
ASP O	349	30.97	-46.23	25.60	:	GLY N	350	29.05	29.05	25.01
GLY CA	350	28.09	-46.70	25.85	:	GLY C	350	28.69	28.69	26.78
GLY O	350	28.77	-44.47	26.45	:	LYS N	351	29.32	29.32	27.84
LYS CA	351	29.71	-45.17	28.84	:	LYS CB	351	30.32	30.32	30.02
LYS CG	351	29.30	-46.71	30.78	:	LYS CD	351	29.72	29.72	32.26
LYS CE	351	29.38	-48.10	32.84	:	LYS NZ	351	29.86	29.86	34.19
LYS C	351	30.65	-44.11	28.38	:	LYS O	351	30.50	30.50	28.92
ASP N	352	31.49	-44.37	27.39	:	ASP CA	352	32.32	32.32	26.84
ASP CB	352	33.29	-43.89	25.84	:	ASP CG	352	34.44	34.44	26.56
ASP OD1	352	34.15	-45.34	27.51	:	ASP OD2	352	35.61	35.61	26.18
ASP C	352	31.52	-42.20	26.17	:	ASP O	352	31.62	31.62	26.47
VAL N	353	30.54	-42.70	25.39	:	VAL CA	353	29.67	29.67	24.57
VAL CB	353	28.67	-42.68	23.76	:	VAL CG1	353	27.96	27.96	22.80
VAL CG2	353	29.40	-43.77	23.00	:	VAL C	353	28.92	28.92	25.56
VAL O	353	28.97	-39.78	25.44	:	LEU N	354	28.33	28.33	26.60
LEU CA	354	27.64	-40.81	27.61	:	LEU CB	354	27.01	27.01	28.63
LEU CG	354	25.69	-42.35	28.30	:	LEU CD1	354	25.00	25.00	29.54
LEU CD2	354	24.73	-41.28	27.84	:	LEU C	354	28.63	28.63	28.28
LEU O	354	28.32	-38.72	28.50	:	GLY N	355	29.86	29.86	28.49
GLY CA	355	30.84	-39.42	29.12	:	GLY C	355	31.21	31.21	28.34
GLY O	355	31.45	-37.10	28.99	:	LEU N	356	31.23	31.23	26.98
LEU CA	356	31.55	-37.08	26.16	:	LEU CB	356	32.10	32.10	24.83

24/32

III 124.

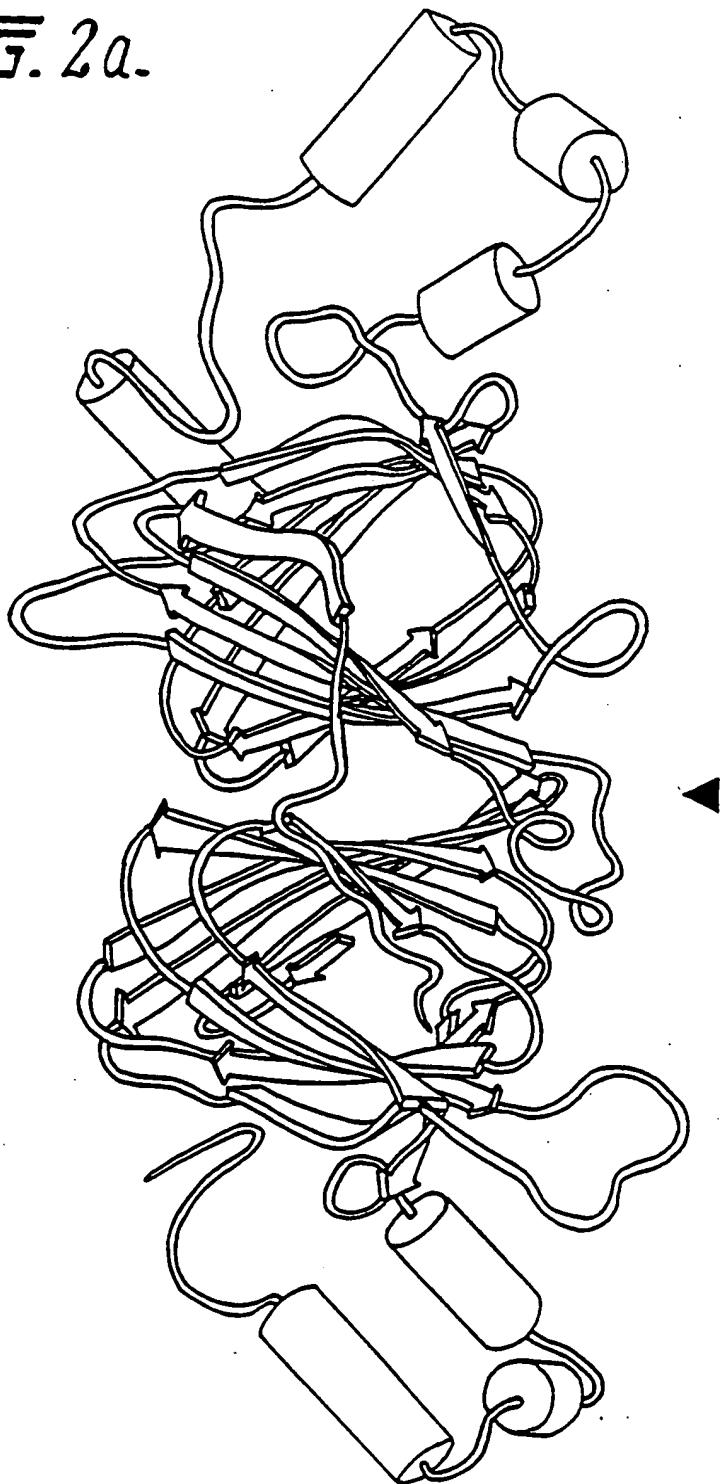
LEU CG 356	33.37	-38.20	24.78	:	LEU CD1 356	33.32	33.32	23.64
LEU CD2 356	34.49	-37.20	24.74	:	LEU C 356	30.27	30.27	25.89
LEU O 356	30.27	-35.10	25.58	:	THR N 357	29.12	29.12	26.01
THR CA 357	27.83	-36.31	25.86	:	THR CB 357	26.70	26.70	25.68
THR OG1 357	26.92	-38.07	24.49	:	THR CG2 357	25.35	25.35	25.58
THR C 357	27.53	-35.47	27.09	:	THR O 357	26.79	26.79	26.87
PHE N 358	28.02	-35.62	28.33	:	PHE CA 358	27.39	27.39	29.47
PHE CB 358	26.47	-35.97	30.09	:	PHE CG 358	25.06	25.06	29.59
PHE CD1 358	24.36	-34.84	29.44	:	PHE CD2 358	24.47	24.47	29.34
PHE CE1 358	23.04	-34.89	29.05	:	PHE CE2 358	23.16	23.16	28.94
PHE CZ 358	22.44	-36.11	28.80	:	PHE C 358	28.24	28.24	30.59
PHE O 358	27.73	-34.15	31.70	:	SER N 359	29.52	29.52	30.46
SER CA 359	30.38	-33.45	31.53	:	SER CB 359	29.74	29.74	32.60
SER OG 359	28.66	-31.61	32.20	:	SER C 359	30.75	30.75	32.29
SER O 359	31.70	-35.39	31.86	:	GLY N 360	29.89	29.89	33.24
GLY CA 360	30.18	-36.17	34.16	:	GLY C 360	30.62	30.62	33.47
GLY O 360	30.41	-37.67	32.29	:	SER N 361	31.29	31.29	34.22
SER CA 361	31.74	-39.47	33.66	:	SER CB 361	32.51	32.51	34.78
SER OG 361	31.66	-40.19	35.95	:	SER C 361	30.59	30.59	33.15
SER O 361	29.51	-40.44	33.77	:	GLY N 362	30.79	30.79	32.08
GLY CA 362	29.83	-42.22	31.71	:	GLY C 362	29.30	29.30	32.90
GLY O 362	28.19	-43.64	32.91	:	ASP N 363	30.08	30.08	33.97
ASP CA 363	29.68	-43.82	35.15	:	ASP CB 363	30.94	30.94	35.85
ASP CG 363	30.95	-45.76	35.56	:	ASP OD1 363	31.71	31.71	34.69
ASP OD2 363	30.09	-46.47	36.16	:	ASP C 363	28.80	28.80	36.09
ASP O 363	27.92	-43.68	36.73	:	GLU N 364	29.17	29.17	36.27
GLU CA 364	28.36	-40.89	37.06	:	GLU CB 364	29.01	29.01	37.10
GLU CG 364	29.84	-39.47	38.34	:	GLU CD 364	30.59	30.59	38.50
GLU OE1 364	30.40	-37.53	39.55	:	GLU OE2 364	31.36	31.36	37.61
GLU C 364	26.95	-40.73	36.45	:	GLU O 364	25.93	25.93	37.14
VAL N 365	26.86	-40.40	35.14	:	VAL CA 365	25.58	25.58	34.51
VAL CB 365	25.75	-39.58	33.07	:	VAL CG1 365	26.75	26.75	32.21
VAL CG2 365	24.43	-39.73	32.35	:	VAL C 365	24.90	24.90	34.47
VAL O 365	23.70	-41.51	34.75	:	MET N 366	25.51	25.51	34.27
MET CA 366	24.71	-43.98	34.29	:	MET CB 366	25.50	25.50	34.01
MET CG 366	25.73	-45.78	32.58	:	MET SD 366	24.18	24.18	31.65
MET CE 366	23.34	-47.27	32.56	:	MET C 366	24.05	24.05	35.66
MET O 366	22.87	-44.55	35.78	:	LYS N 367	24.80	24.80	36.71
LYS CA 367	24.41	-44.04	38.09	:	LYS CB 367	25.51	25.51	39.03
LYS CG 367	26.21	-44.63	39.88	:	LYS CD 367	27.21	27.21	39.04
LYS CE 367	28.63	-45.39	39.71	:	LYS NZ 367	29.74	29.74	38.73
LYS C 367	23.15	-43.27	38.42	:	LYS O 367	22.15	22.15	38.91
LEU N 368	23.23	-41.99	38.09	:	LEU CA 368	22.13	22.13	38.34
LEU CB 368	22.56	-39.70	37.96	:	LEU CG 368	21.53	21.53	37.67
LEU CD1 368	21.08	-37.93	38.94	:	LEU CD2 368	22.17	22.17	36.66
LEU C 368	20.93	-41.47	37.50	:	LEU O 368	19.80	19.80	38.01
ILE N 369	21.17	-42.00	36.29	:	ILE CA 369	20.06	20.06	35.42
ILE CB 369	20.67	-42.72	34.00	:	ILE CG2 369	19.88	19.88	33.20
ILE CG1 369	20.72	-41.40	33.22	:	ILE CD1 369	19.35	19.35	32.98
ILE C 369	19.38	-43.54	36.14	:	ILE O 369	18.16	18.16	36.31
ASN N 370	20.22	-44.40	36.69	:	ASN CA 370	19.67	19.67	37.50
ASN CB 370	20.75	-46.52	37.64	:	ASN CG 370	20.60	20.60	36.39
ASN OD1 370	21.46	-47.53	35.50	:	ASN ND2 370	19.41	19.41	36.22
ASN C 370	19.07	-45.03	38.86	:	ASN O 370	18.37	18.37	39.40
LYS N 371	19.21	-43.82	39.43	:	LYS CA 371	18.56	18.56	40.72
LYS CB 371	18.79	-42.03	41.22	:	LYS CG 371	20.26	20.26	41.48
LYS CD 371	20.31	-40.52	42.58	:	LYS CE 371	21.71	21.71	42.92
LYS NZ 371	22.07	-38.78	42.07	:	LYS C 371	17.04	17.04	40.81
LYS O 371	16.53	-43.99	41.88	:	GLN N 372	16.31	16.31	39.70

25|32

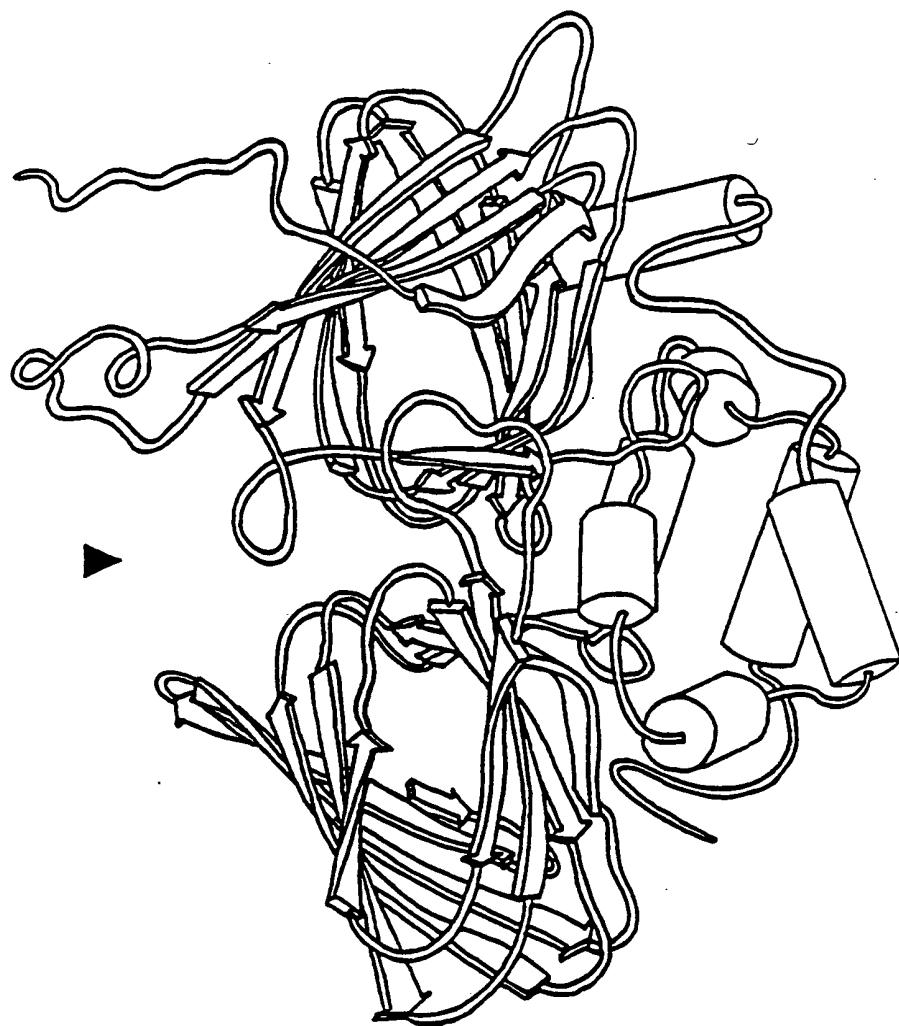
III 1.25.

GLN CA 372	14.85	-43.40	39.69	:	GLN CB 372	14.36	14.36	38.33
GLN CG 372	12.85	-42.91	38.06	:	GLN CD 372	11.94	11.94	39.08
GLN OE1 372	11.26	-43.03	39.74	:	GLN NE2 372	11.83	11.83	39.23
GLN C 372	14.09	-44.64	40.08	:	GLN O 372	13.65	13.65	41.23
SER N 373	13.81	-45.64	39.24	:	SER CA 373	13.16	13.16	39.59
SER CB 373	13.05	-47.30	41.11	:	SER OG 373	12.07	12.07	41.85
SER C 373	11.75	-46.91	39.10	:	SER O 373	11.28	11.28	38.67
GLY N 374	11.14	-45.73	39.18	:	GLY CA 374	9.82	9.82	38.63
GLY C 374	9.85	-45.66	37.11	:	GLY O 374	10.92	10.92	36.48
SER N 375	8.69	-45.82	36.53	:	SER CA 375	8.63	8.63	35.10
SER CB 375	8.60	-47.31	34.67	:	SER OG 375	9.83	9.83	34.93
SER C 375	7.40	-45.13	34.60	:	SER O 375	6.30	6.30	35.11
TYR N 376	7.59	-44.29	33.60	:	TYR CA 376	6.57	6.57	32.95
TYR CB 376	5.47	-44.40	32.40	:	TYR CG 376	5.78	5.78	31.00
TYR CD1 376	6.82	-45.79	30.73	:	TYR CE1 376	7.09	7.09	29.46
TYR CD2 376	4.97	-44.53	29.98	:	TYR CE2 376	5.21	5.21	28.69
TYR CZ 376	6.27	-45.78	28.45	:	TYR OH 376	6.51	6.51	27.15
TYR C 376	5.99	-42.49	33.92	:	TYR O 376	6.48	6.48	33.94
PHE N 377	5.01	-42.81	34.74	:	PHE CA 377	4.44	4.44	35.61
PHE CB 377	2.97	-42.10	35.76	:	PHE CG 377	2.31	2.31	34.41
PHE CD1 377	2.13	-43.48	33.89	:	PHE CD2 377	1.91	1.91	33.71
PHE CE1 377	1.54	-43.62	32.67	:	PHE CE2 377	1.34	1.34	32.49
PHE CZ 377	1.15	-42.51	31.97	:	PHE C 377	5.21	5.21	36.91
PHE O 377	5.66	-42.97	37.33	:	VAL N 378	5.41	5.41	37.57
VAL CA 378	6.26	-40.66	38.74	:	VAL CB 378	7.61	7.61	38.10
VAL CG1 378	8.25	-39.09	38.78	:	VAL CG2 378	8.55	8.55	38.18
VAL C 378	5.65	-39.65	39.73	:	VAL O 378	4.96	4.96	39.34
ASP N 379	5.91	-39.84	41.01	:	ASP CA 379	5.44	5.44	42.06
ASP CB 379	5.80	-39.55	43.36	:	ASP CG 379	5.13	5.13	44.54
ASP OD1 379	5.57	-39.19	45.67	:	ASP OD2 379	4.18	4.18	44.35
ASP C 379	6.17	-37.63	41.94	:	ASP O 379	7.41	7.41	41.87
ALA N 380	5.55	-36.42	41.94	:	ALA CA 380	6.34	6.34	41.62
ALA CB 380	6.54	-35.06	40.13	:	ALA C 380	5.94	5.94	42.07
ALA OT1 380	4.96	-33.32	41.55	:	ALA OT2 380	6.68	6.68	42.84

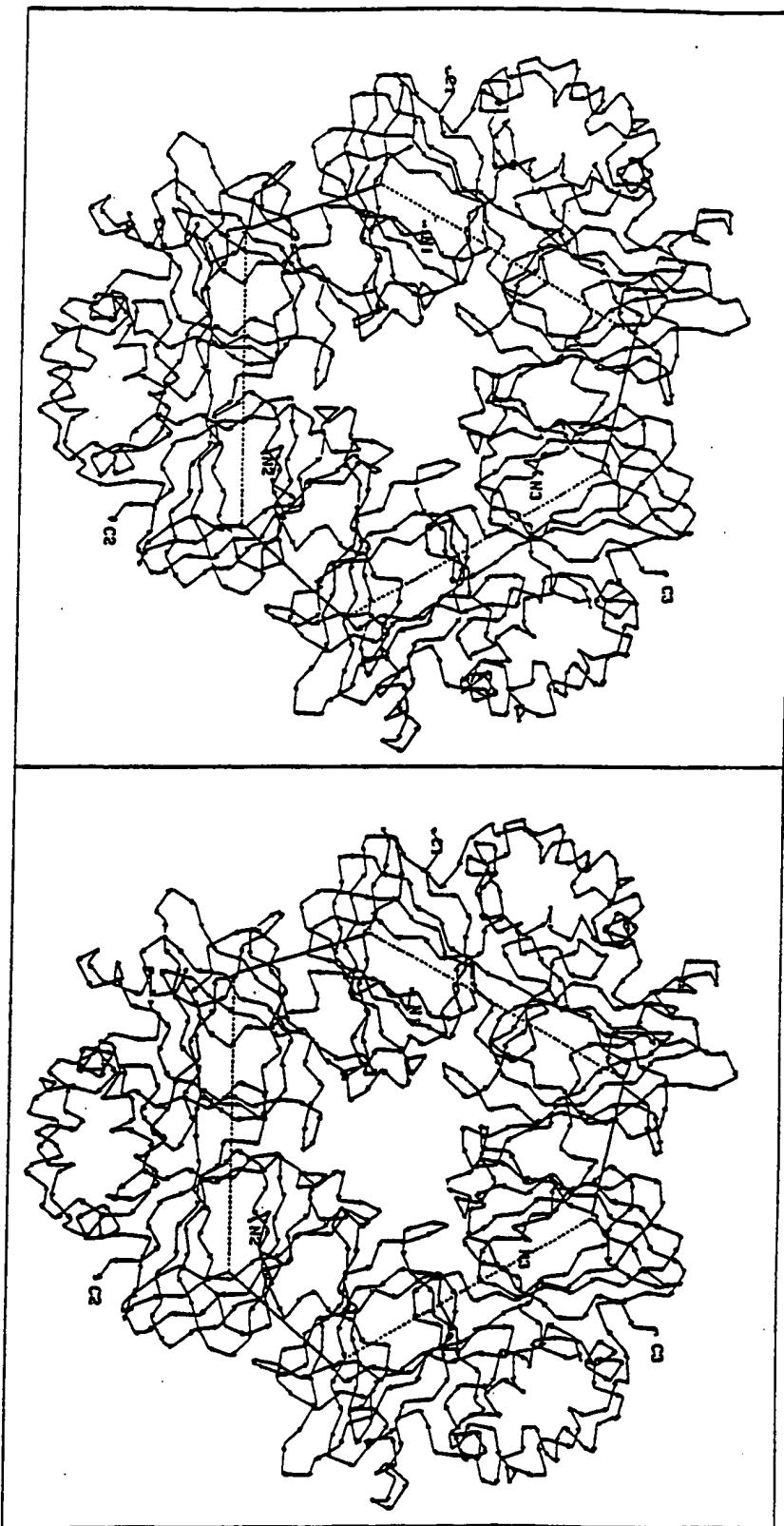
26/32

FIG. 2a.

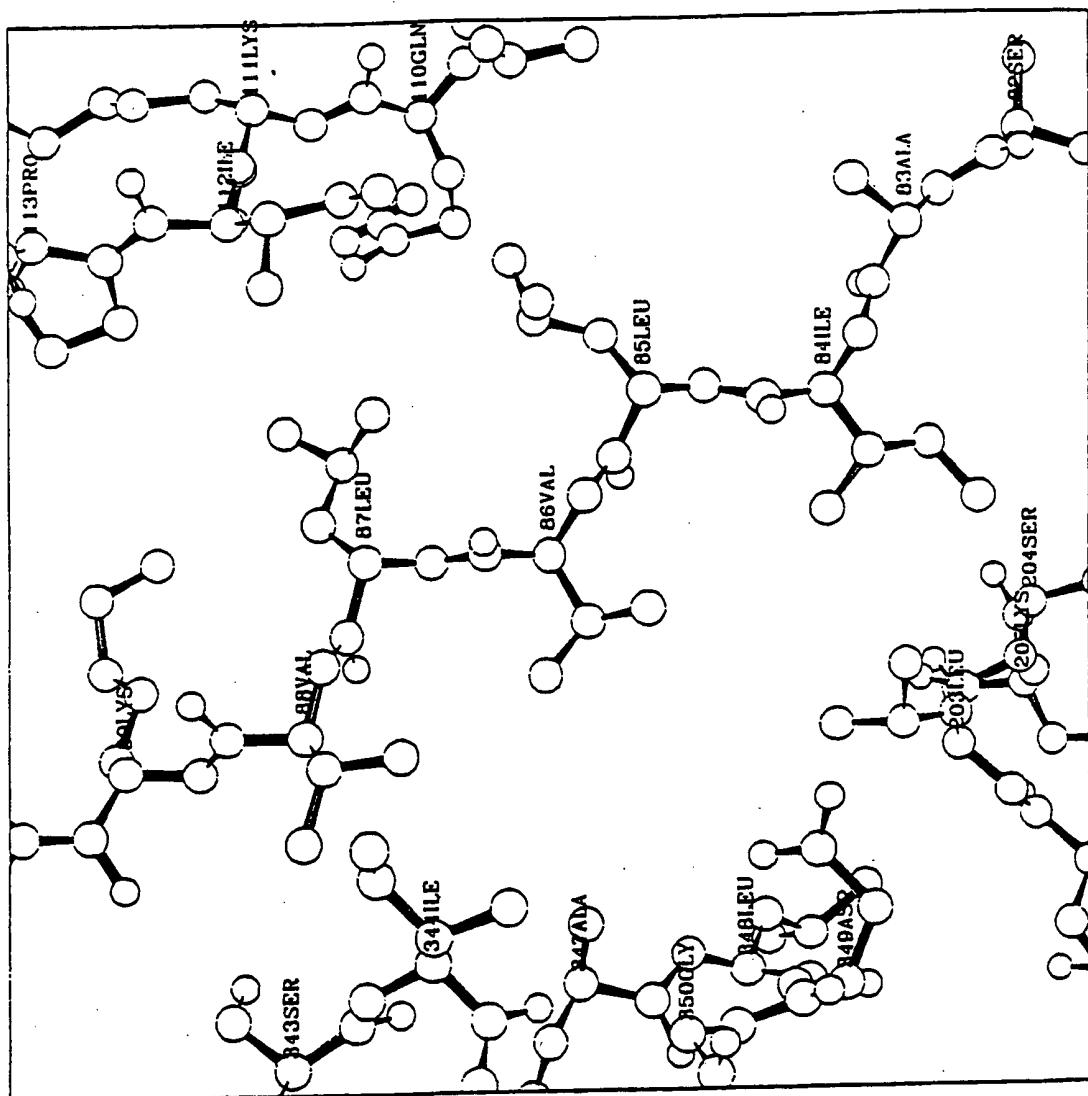
27/32

FIG. 2b.

28/32

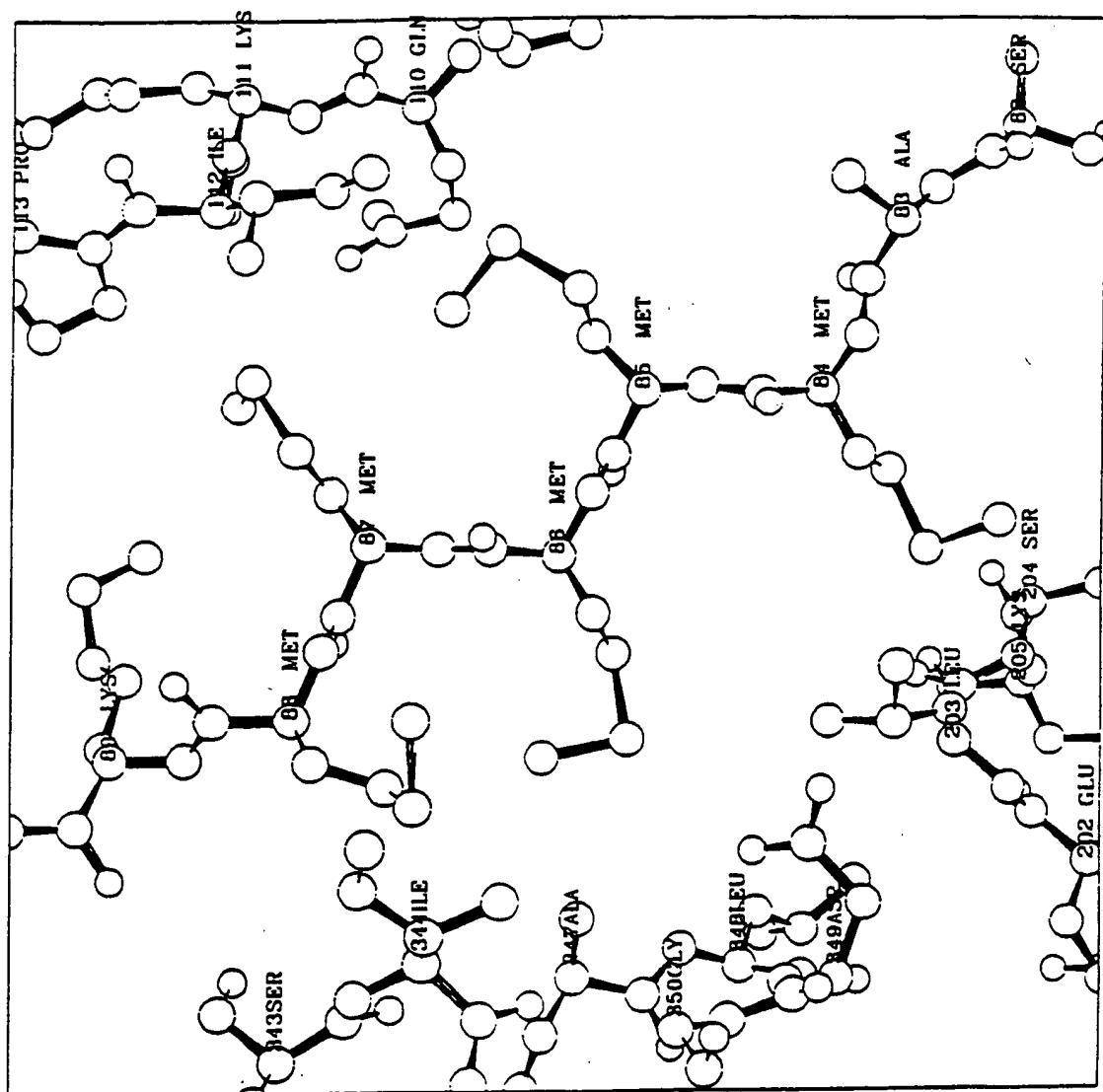
III. 3.

29 | 32



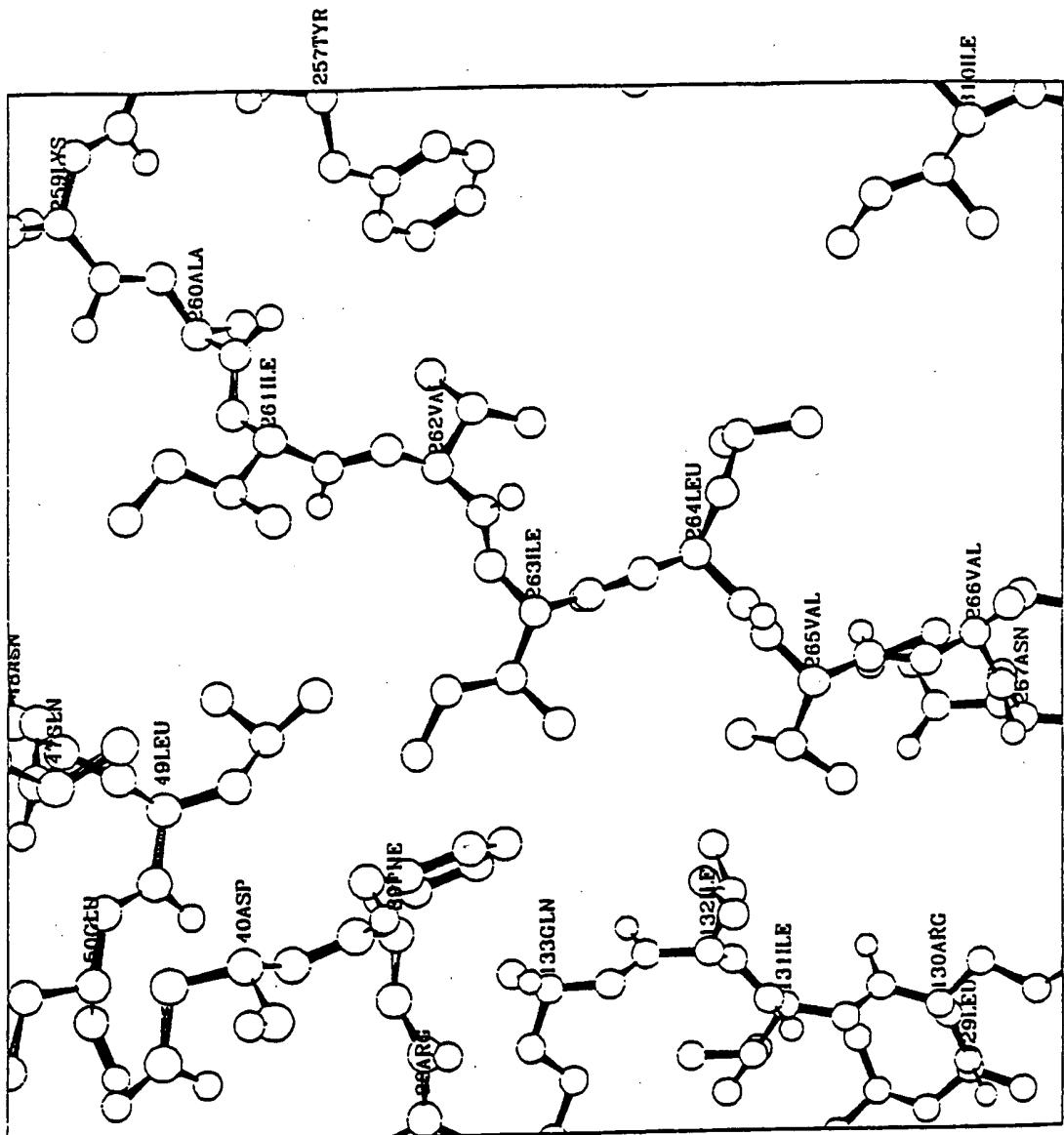
III. 4A.

30/32



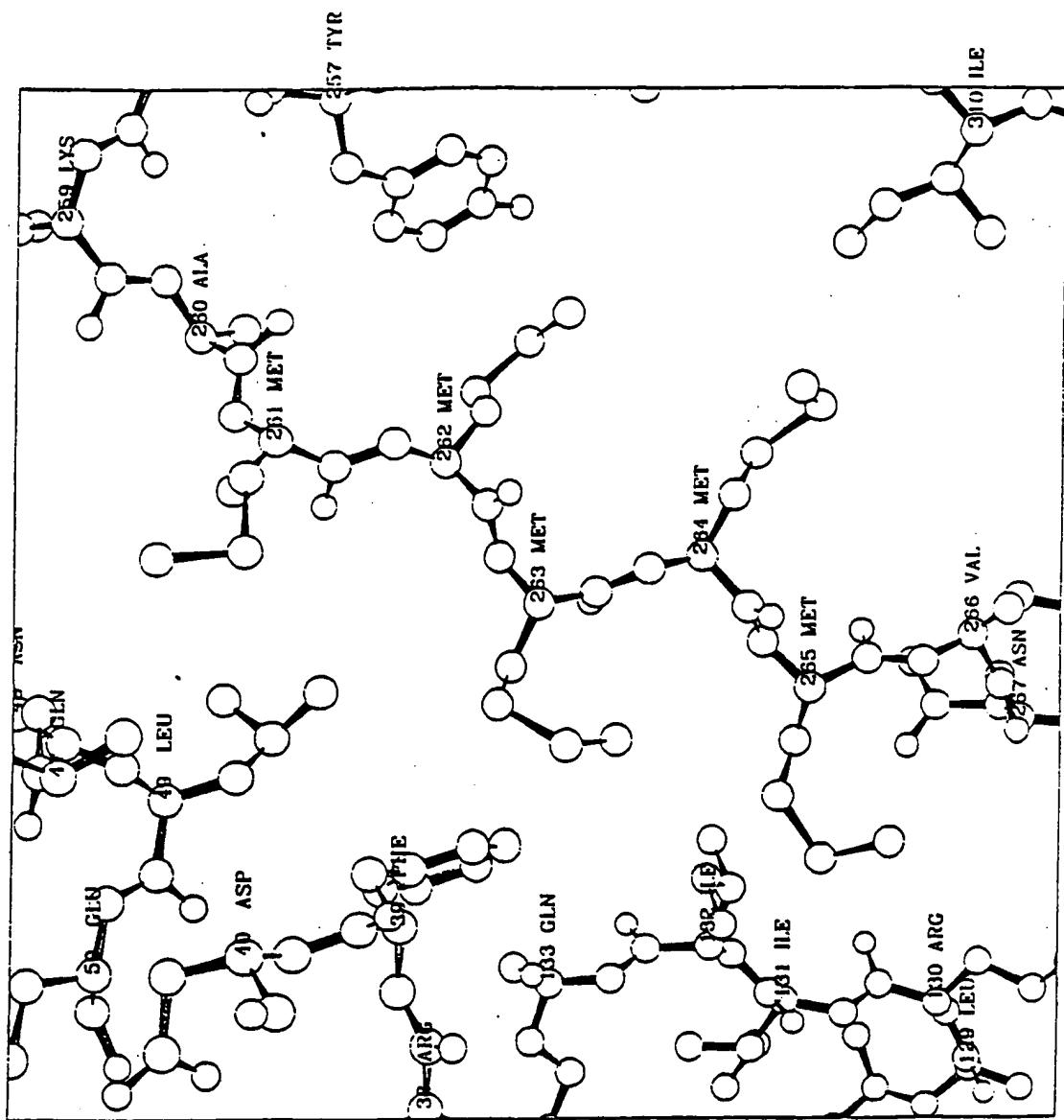
III.4B.

31/32



III. 5A.

32/32

III. 5B.

## INTERNATIONAL SEARCH REPORT

International Application No. PCT/AU 90/00430

## I. CLASSIFICATION OF SUBJECT MATTER (if several classification symbols apply, indicate all) 6

According to International Patent Classification (IPC) or to both National Classification and IPC

Int. Cl. <sup>5</sup> C07K 13/00, C12N 15/29, A01H 5/00, A01H 5/10, 1/00, C12N 1/21 // (C12N 1/21, C12R 1:01)

## II. FIELDS SEARCHED

Minimum Documentation Searched 7

4

## Classification System

## Classification Symbols

IPC

WPAT, USPM DERVENT DATABASE KEYWORDS: SEED STORAGE PROTEIN

7

Documentation Searched other than Minimum Documentation  
to the Extent that such Documents are Included in the Fields Searched 8AU: C12N 15/29, C07K 13/00; CHEMICAL ABSTRACTS KEYWORDS AS ABOVE AND BIOTECHNOLOGY DERVENT  
DATABASE KEYWORDS AS ABOVE, ADDITIONAL KEYWORDS: MUTEIN, MUTANT, VARIANT, MODIFIED,  
MODIFICATION

## III. DOCUMENTS CONSIDERED TO BE RELEVANT 9

Category*	Citation of Document, " with indication, where appropriate, of the relevant passages 12	Relevant to Claim No 13
P,A	Protein Engineering, volume 3, no. 8, 1990, pp. 725-731, Chan-Shick Kim <u>et al.</u> , "Improvement of nutritional value and functional properties of soybean glycinin by protein engineering, "whole document.	(1-13)
A	Plant Molecular Biology, vol 11, 1988, pp. 717-729, L.M. Hoffman <u>et al.</u> , "A modified storage protein is synthesized, processed, and degraded in the seeds of transgenic plants", whole document.	(1-16)
A	Biochem. Physiol. Pflanzen, 183, 1988 pp. 211-218, Gerhard Saalbach <u>et al.</u> , "Construction of storage protein genes with increased number of methionine codons and their use in transformation experiments", whole document.	(1-16)

(continued)

\* Special categories of cited documents: 10

- "A" document defining the general state of the art which is not considered to be of particular relevance
- "E" earlier document but published on or after the international filing date
- "L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
- "O" document referring to an oral disclosure, use, exhibition or other means
- "P" document published prior to the international filing date but later than the priority date claimed
- "T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
- "X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step
- "Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.
- "Z" document member of the same patent family

8

## IV. CERTIFICATION

Date of the Actual Completion of the International Search 3 January 1991 (03.01.91)	Date of Mailing of this International Search Report 10 January 1991
International Searching Authority Australian Patent Office	Signature of Authorized Officer M.E. KEESE

## FURTHER INFORMATION CONTINUED FROM THE SECOND SHEET

A	Nature, volume 339, 29 June 1989, pp. 658-659, Dagmar Ringe, "The sheep in wolf's clothing", whole document.	(1-13)
A	Fed. Proc. Fed. Am. Soc. Exptl. Biol; vol 46, 6, p. 2023 C.D. Dickinson <i>et al.</i> , "Engineering of soybean seed storage proteins", abstract.	(1-13)

## V. [ ] OBSERVATIONS WHERE CERTAIN CLAIMS WERE FOUND UNSEARCHABLE 1

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. [ ] Claim numbers ..., because they relate to subject matter not required to be searched by this Authority, namely:

2. [ ] Claim numbers ..., because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

3. [ ] Claim numbers ..., because they are dependent claims and are not drafted in accordance with the second and third sentences of PCT Rule 6.4 (a):

## VI. [ ] OBSERVATIONS WHERE UNITY OF INVENTION IS LACKING 2

This International Searching Authority found multiple inventions in this international application as follows:

1. [ ] As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims of the international application.

2. [ ] As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims of the international application for which fees were paid, specifically claims:

3. [ ] No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claim numbers:

4. [ ] As all searchable claims could be searched without effort justifying an additional fee, the International Searching Authority did not invite payment of any additional fee.

## | Remark on Protest

| [ ] The additional search fees were accompanied by applicant's protest.

| [ ] No protest accompanied the payment of additional search fees.

This Page Blank (uspto)